**The Mechanism of Selective Ammoxidation of Propene to Acrylonitrile on Bismuth Molybdates from Quantum Mechanical Calculations**

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Gas Phase Energy, Zero Point Energy, and Coordinates for all compounds mentioned in the manuscript:

## Ammoxidation of allyl on $Mo3O_8(NH)$ – Figure 4

**1**

Energy = -860.038280 hartree
Zero Point Energy (ZPE): 26.172 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.8422109880 | 0.6708402985 | 0.9520967338 |
| O2 | -1.0322554050 | 0.7087909867 | 1.5730401689 |
| O3 | -3.5045761123 | 2.2410961270 | 0.9586253535 |
| O4 | -3.7359571187 | -0.4376228156 | 2.2168110571 |
| O5 | -2.9736392953 | 0.0497924886 | -0.6273646806 |
| Mo6 | -3.4322929483 | -0.5634100064 | 4.1190380981 |
| O7 | -1.5077492227 | -0.5385743759 | 4.2665046139 |
| Mo8 | -0.2665430753 | 0.5523789704 | 3.3201013156 |
| O9 | -4.1543059183 | -1.9225435623 | 4.8375737726 |
| O10 | -0.1386370907 | 2.0863561916 | 4.0516850406 |
| O11 | 1.2847635175 | -0.1477344252 | 3.2889117075 |
| N12 | -4.0549446293 | 0.8938568287 | 4.8677771365 |
| H13 | -4.7112446783 | 1.1790420904 | 5.5959485203 |

**2**

Energy = -977.367193 hartrees
Zero Point Energy (ZPE): 72.472 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9133866878 |
| O3 | 1.5712925038 | 0.0000000000 | -0.6643202141 |
| O4 | -0.9780025941 | 1.5310305106 | -0.4969989882 |
| O5 | -0.8544655879 | -1.3790021649 | -0.5590191447 |
| Mo6 | -2.7221545479 | 2.2183577602 | 0.0452407126 |
| O7 | -2.5915173190 | 1.5027332656 | 1.8482856295 |
| Mo8 | -1.4739340312 | 0.5348451111 | 3.0196679085 |
| O9 | -2.7535520289 | 3.9123804535 | 0.0059629972 |

| | | | |
|---|---|---|---|
| N10 | -4.1266917904 | 1.2922202785 | -0.8868032212 |
| H11 | -4.8829107630 | 1.8218778786 | -1.3217513930 |
| C12 | -5.5576812964 | -0.6343362575 | -0.3097955097 |
| C13 | -4.3149150715 | -0.1684740768 | -1.0217955864 |
| H14 | -3.4244873980 | -0.6668810340 | -0.6195530650 |
| H15 | -4.3625051201 | -0.4169234855 | -2.0895182287 |
| C16 | -6.5793372761 | -1.2357814700 | -0.9198763392 |
| H17 | -6.5769871864 | -1.4252118353 | -1.9909921906 |
| H18 | -7.4485229370 | -1.5779134785 | -0.3662542034 |
| H19 | -5.5790817322 | -0.4624606018 | 0.7653614354 |
| O20 | -2.3196740616 | -0.8204687059 | 3.6262284717 |
| O21 | -0.9550410604 | 1.4838209414 | 4.3388802435 |

**TS1**

Energy = -977.313921 hartrees

Zero Point Energy (ZPE): 68.671 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1950658411 | 0.4242367575 | 0.1071557207 |
| O2 | -0.0301751128 | -0.1061635633 | 1.9095735576 |
| O3 | 1.8046661077 | 0.6289609766 | -0.4004838024 |
| O4 | -0.7185635114 | 2.0351480391 | 0.0351931059 |
| O5 | -0.7257568739 | -0.7485624846 | -0.9408581175 |
| Mo6 | -2.6981969931 | 2.1211820605 | -0.0725297086 |
| H7 | -1.7891561845 | -0.6574580548 | -1.3274122064 |
| C8 | -3.2648055201 | -0.4975366110 | -1.4952115746 |
| O9 | -3.1853054134 | 3.7126601911 | -0.3866848764 |
| N10 | -3.5293682704 | 0.8514449832 | -1.3348885933 |
| C11 | -3.5979872751 | -1.1822791237 | -2.7445059955 |
| Mo12 | -1.7322403913 | 0.1307349414 | 2.8286306897 |
| H13 | -3.3794439955 | -1.0675376063 | -0.5689600811 |
| O14 | -2.8068033414 | 1.0340572511 | 1.5927968418 |
| C15 | -3.7134668089 | -0.6123506698 | -3.9561347396 |
| H16 | -3.5423172794 | 0.4482620458 | -4.1268231026 |
| H17 | -3.9667750039 | -1.2019044209 | -4.8297985907 |
| H18 | -3.7184092804 | -2.2597925765 | -2.6518316364 |
| O19 | -1.5358861460 | 1.0199448751 | 4.2726257828 |
| O20 | -2.4160837035 | -1.3919574904 | 3.2043865359 |
| H21 | -4.0051905228 | 1.2677224463 | -2.1390211985 |

**3**

Energy = -977.353358

Zero Point Energy (ZPE): 71.566 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.9704622906 | 0.4345165894 | -0.4356431218 |
| O2 | 2.5930369997 | -0.5010674207 | -0.0594599617 |
| O3 | 1.1956929184 | 2.1146811312 | -0.3573321367 |

| | | | |
|---|---|---|---|
| O4 | -0.0360770512 | -0.0163276289 | 1.1571186205 |
| O5 | 0.1203534498 | -0.3978853318 | -1.9287130349 |
| Mo6 | 0.0495967908 | -1.0708035044 | 2.7447962864 |
| O7 | 2.0185390905 | -1.3809561191 | 2.7084813439 |
| Mo8 | 2.8762846660 | -1.9602292169 | 1.1743800660 |
| O9 | -0.4933406052 | -0.5992446377 | 4.2811645461 |
| N10 | -0.1966196142 | -3.1471412526 | 2.6228878706 |
| C11 | -1.0734392240 | -3.8684984906 | 4.7692984163 |
| C12 | -0.5742395238 | -4.0930946731 | 3.4319001472 |
| H13 | -0.4975759725 | -5.1246952481 | 3.0846339872 |
| C14 | -1.4298046115 | -4.8870755480 | 5.5705211946 |
| H15 | -1.3648246791 | -5.9218529468 | 5.2438989271 |
| H16 | -1.7917173449 | -4.7136331671 | 6.5783666843 |
| H17 | -1.1338828020 | -2.8389791319 | 5.1130697527 |
| O18 | 4.5227396163 | -2.3540866032 | 1.4432552469 |
| O19 | 1.9399621495 | -3.3133952697 | 0.6090123584 |
| H20 | -0.0856597574 | 0.0838888911 | -2.7432590630 |
| H21 | 0.2155247594 | -3.4989349780 | 1.7484848484 |

**3** (second isomer)
Energy = -977.349313
Zero Point Energy (ZPE): 71.213 kca/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.3651001004 | 1.6846456960 | 1.1176283155 |
| O2 | -0.9463931105 | 1.3635076245 | 2.3724718523 |
| O3 | -2.8433512266 | 3.3091932273 | 1.0313156849 |
| O4 | -3.6376728328 | 0.8028755423 | 2.2065623295 |
| O5 | -2.0426439968 | 0.6354346090 | -0.4524504509 |
| Mo6 | -3.8387557291 | -0.4459234033 | 3.6313247290 |
| O7 | -2.0067920821 | -0.5676743475 | 4.3247576894 |
| Mo8 | -0.4250817286 | -0.1651505669 | 3.3800856520 |
| O9 | -5.0199130872 | -0.1180871542 | 4.8072352222 |
| N10 | -3.8864063973 | -2.4329444216 | 2.9100203977 |
| C11 | -3.0289169790 | -4.5304577563 | 2.0174794352 |
| C12 | -2.9098041339 | -3.1508763677 | 2.4233391041 |
| H13 | -1.9347117582 | -2.6713263728 | 2.3155295558 |
| C14 | -1.9663001324 | -5.2083352631 | 1.5454875159 |
| H15 | -0.9947441222 | -4.7316481868 | 1.4464622781 |
| H16 | -2.0411471651 | -6.2503866403 | 1.2533956288 |
| H17 | -4.0002188305 | -5.0135937416 | 2.1175138658 |
| O18 | 0.9097481921 | 0.1160148993 | 4.4186663262 |
| O19 | -0.1511578676 | -1.4937908567 | 2.2961607470 |
| H20 | -2.0140441188 | 1.0361491009 | -1.3332038925 |
| H21 | -4.7742875619 | -2.9318797647 | 2.9846921513 |

**TS2**

Energy = -977.331651

Zero Point Energy (ZPE): 69.176 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.4912275262 | 0.4502114856 | -0.0608419326 |
| O2 | 2.4277407160 | -0.0152783029 | 0.1434549514 |
| O3 | -0.0295779230 | 1.8389770141 | -0.8840540031 |
| O4 | -0.0060033031 | 0.1466183018 | 1.8525837842 |
| O5 | -0.0792258805 | -1.5375914940 | -0.5301519280 |
| Mo6 | 0.3743912530 | -1.3846592944 | 2.8504392104 |
| O7 | 2.2045492972 | -1.8432383517 | 2.4543673940 |
| Mo8 | 3.0684891599 | -1.6584640910 | 0.7467212659 |
| O9 | -0.2039596002 | -1.5701069778 | 4.4419859939 |
| N10 | -0.6499839220 | -2.6275318674 | 1.6540029507 |
| C11 | -1.8814213784 | -4.1898901403 | 3.0869349531 |
| C12 | -1.4451676240 | -3.6308899982 | 1.8196138129 |
| H13 | -1.8321922938 | -4.1175851196 | 0.9160823041 |
| C14 | -2.6992204575 | -5.2545632639 | 3.1343424123 |
| H15 | -3.0664979792 | -5.7305555686 | 2.2284508018 |
| H16 | -3.0229171544 | -5.6812424944 | 4.0777261356 |
| H17 | -1.5196449140 | -3.7165906045 | 3.9963870960 |
| O18 | 4.7738135637 | -1.7241022943 | 0.8394959572 |
| O19 | 2.4532028295 | -2.8744831884 | -0.3261756973 |
| H20 | 0.6287247194 | -2.0772532558 | -0.9344193332 |
| H21 | -0.4032355215 | -2.1218907164 | 0.4148300523 |

**4**

Energy = -977.335506h

Zero Point Energy (ZPE): 71.284 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0555784386 | 0.0547561870 | 0.0639664527 |
| O2 | 2.0462112444 | 0.0146249752 | 0.0580208483 |
| O3 | -0.9073853264 | 1.4460854825 | 0.1001435012 |
| O4 | -0.2676655615 | -1.3444295302 | 1.4135461446 |
| O5 | -0.1046759914 | -1.5000069129 | -1.4624166084 |
| Mo6 | 0.5656052901 | -3.0195572886 | 1.5523499263 |
| O7 | 2.4166758298 | -2.7444451019 | 1.0282826509 |
| Mo8 | 3.0593600622 | -1.5241996240 | -0.2876866916 |
| O9 | 0.1649627076 | -4.0525202769 | 2.8446205970 |
| N10 | -0.2774043838 | -3.8033978658 | -0.0330914710 |
| C11 | -1.3653204373 | -5.3740945272 | -1.5110559549 |
| C12 | -0.9060171427 | -4.9156244088 | -0.2108245343 |
| H13 | -1.1151843042 | -5.5744887678 | 0.6431911392 |
| C14 | -2.0064793964 | -6.5448603999 | -1.6638881532 |
| H15 | -2.2114653528 | -7.1924636291 | -0.8151618468 |

| | | | |
|---|---|---|---|
| H16 | -2.3407866363 | -6.8895818263 | -2.6364626367 |
| H17 | -1.1575940058 | -4.7312589057 | -2.3635519547 |
| O18 | 4.7471453696 | -1.2749640725 | -0.2076383412 |
| O19 | 2.5735464708 | -2.0799929499 | -1.8630513007 |
| H20 | 0.7235659210 | -1.6166323209 | -1.9835223813 |
| H21 | -0.2766778775 | -2.4205010823 | -1.0658311114 |

**4** (another conformer)
Energy = -977.334010
Zero Point Energy (ZPE): 71.481 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9876201921 |
| O3 | 1.3806602451 | 0.0000000000 | -0.9802138943 |
| O4 | -1.3402884836 | 1.4185999490 | -0.2833116590 |
| O5 | -1.6253789023 | -1.4477133358 | -0.1387922959 |
| Mo6 | -2.9928774876 | 1.6219236195 | 0.5779674357 |
| O7 | -2.7083185584 | 1.0691620120 | 2.4159908118 |
| Mo8 | -1.5266124981 | -0.2956185518 | 3.0350175059 |
| O9 | -3.9401223492 | 2.9965351936 | 0.2385024321 |
| N10 | -3.8493663420 | 0.0661417953 | -0.2569272336 |
| C11 | -5.9862742006 | 0.7830040953 | -1.2278231110 |
| C12 | -4.9604158020 | -0.1823949816 | -0.8642034597 |
| H13 | -5.1621786895 | -1.2254936334 | -1.1416487676 |
| C14 | -7.1177768962 | 0.4069744078 | -1.8494157065 |
| H15 | -7.3075979611 | -0.6326976633 | -2.1052983179 |
| H16 | -7.8860557071 | 1.1259987015 | -2.1171449330 |
| H17 | -5.8039247182 | 1.8242010242 | -0.9734173137 |
| O18 | -1.2389160407 | -0.2257866889 | 4.7172121528 |
| O19 | -2.1488097959 | -1.8482930574 | 2.5579247054 |
| H20 | -1.7450216488 | -1.9771375115 | 0.6827105623 |
| H21 | -2.5298546065 | -0.9924741805 | -0.2727720491 |

**TS3**
Energy = -977.271986 hartrees
Zero Point Energy (ZPE): 75.488 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.5625241853 | 0.6312867718 | 0.0279946327 |
| O2 | 2.3996940561 | -0.1313454187 | -0.0906743898 |
| O3 | 0.2890814324 | 2.1365888577 | -0.6988212458 |
| O4 | -0.1078996222 | 0.0517955421 | 1.7425625490 |
| O5 | 0.1256529064 | -1.0118969125 | -1.3085819765 |
| Mo6 | 0.4232915311 | -1.4290335226 | 2.8656158362 |

| | | | |
|---|---|---|---|
| O7 | 2.2438328741 | -1.6563057177 | 2.3499374036 |
| Mo8 | 2.9210088176 | -1.7970599431 | 0.5491196268 |
| O9 | 0.1947912912 | -1.5311240629 | 4.5480732630 |
| N10 | -0.4508578238 | -2.9709524652 | 2.0932769237 |
| C11 | -1.4138047472 | -4.3725736514 | 0.3616873175 |
| C12 | -0.3346006538 | -3.7094213947 | 1.0881922544 |
| H13 | 0.8987500287 | -3.4851181992 | 0.3191349254 |
| C14 | -1.1578799788 | -5.1077558990 | -0.7326079214 |
| H15 | -0.1442678231 | -5.2295208865 | -1.1036379573 |
| H16 | -1.9530880173 | -5.6074403690 | -1.2776792996 |
| H17 | -2.4270839662 | -4.2560153598 | 0.7415845584 |
| O18 | 4.5175574886 | -2.3766908107 | 0.3674210088 |
| O19 | 1.6103032262 | -2.8869475038 | -0.3328528206 |
| H20 | 0.7082133300 | -1.8223110019 | -1.0778495390 |
| H21 | -0.7922828764 | -1.3074531093 | -1.3799547201 |

**5**

Energy = -977.300110 hartrees
Zero Point Energy (ZPE): 68.921 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.1630865439 | 1.4341640451 | 1.3228876041 |
| O2 | -1.6398015835 | 1.9933890560 | 2.3002358943 |
| O3 | -4.1908164551 | 2.7053430326 | 0.8428598885 |
| O4 | -3.8214790876 | 0.0283866054 | 2.3264289819 |
| O5 | -1.7476675155 | 0.7729798714 | -0.1497191180 |
| Mo6 | -3.0977924982 | -1.1285655723 | 3.7840466713 |
| O7 | -1.4425199827 | -0.2876648370 | 4.0806396435 |
| Mo8 | -0.2331519692 | 0.9339384627 | 3.1298596092 |
| O9 | -4.2411796406 | -1.4807284008 | 4.9960046775 |
| N10 | -2.9814799184 | -2.8030904665 | 2.6035807716 |
| C11 | -3.0234336589 | -5.1058583608 | 1.4328807073 |
| C12 | -3.0109836721 | -3.8457307943 | 2.0670247174 |
| C13 | -3.8745731788 | -6.0966522451 | 1.7646039519 |
| H14 | -4.6089975153 | -5.9837971776 | 2.5544547745 |
| H15 | -3.8411156104 | -7.0425913769 | 1.2370471025 |
| H16 | -2.2894282397 | -5.2309113285 | 0.6402463725 |
| O17 | 1.0304025367 | 1.7167400738 | 3.9680401991 |
| O18 | 0.1286900878 | 0.0966533625 | 1.2876445161 |
| H19 | -2.0265914021 | 0.1320819026 | -0.8151590080 |
| H20 | -0.8654981514 | 0.4450913401 | 0.3462622419 |
| H21 | 0.6855377793 | -0.6867969020 | 1.2136591704136591704 |

**TS4**

Energy = -977.322669 hartrees
Zero Point Energy (ZPE): 67.602 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -1.7808658395 | 2.1816924691 | 1.5932433278 |
| O2 | -0.3993294294 | 0.9801873956 | 2.3464153734 |
| O3 | -1.7644385718 | 3.7272261483 | 2.2843331393 |
| O4 | -3.2536969625 | 1.2755110098 | 2.3824066082 |
| O5 | -1.8182924933 | 1.8621030537 | -0.2940182955 |
| Mo6 | -4.0638456897 | -0.1924411644 | 3.2483768478 |
| O7 | -2.2985734709 | -0.6218414246 | 4.1331086293 |
| Mo8 | -0.7903704320 | -0.6996880559 | 3.0950662809 |
| O9 | -5.3615459296 | -0.0025750187 | 4.3337897485 |
| N10 | -3.9000731754 | -1.9045699622 | 2.1663975878 |
| C11 | -4.2583763984 | -4.1177444265 | 1.2556521894 |
| C12 | -4.6528143642 | -2.9426866297 | 2.0180502711 |
| H13 | -5.6453446553 | -2.9840220626 | 2.4870274699 |
| C14 | -5.0581669535 | -5.1918347156 | 1.1476146582 |
| H15 | -6.0361792894 | -5.2207391774 | 1.6221756312 |
| H16 | -4.7604628419 | -6.0713517598 | 0.5870004195 |
| H17 | -3.2780078006 | -4.0951606498 | 0.7844884891 |
| O18 | 0.5532645386 | -1.3229577434 | 3.9339954480 |
| O19 | -1.4048987651 | -1.8148889136 | 1.7759521771 |
| H20 | -1.6719452515 | 2.5614722600 | -0.9471577446 |
| H21 | -2.5274437639 | -1.9384641462 | 1.8043265663 |

**7**

Energy = -977.331161 hartrees

Zero Point Energy (ZPE): 69.573 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -1.8819619546 | 2.0675228846 | 1.4240292345 |
| O2 | -0.6336449108 | 0.9564278630 | 2.3691417363 |
| O3 | -1.7254374010 | 3.6785798665 | 1.9305026596 |
| O4 | -3.5175620773 | 1.4087872445 | 2.1925136930 |
| O5 | -1.8261208109 | 1.5493805731 | -0.4136038322 |
| Mo6 | -3.9934474775 | -0.1110259724 | 3.2618143705 |
| O7 | -2.3718169230 | -0.5569260756 | 4.1570544520 |
| Mo8 | -0.6738035545 | -0.7249679498 | 3.3009388829 |
| O9 | -5.3843967464 | -0.0482975250 | 4.2428118867 |
| N10 | -4.1291229413 | -1.6776575126 | 2.1419605906 |
| C11 | -4.9079615865 | -3.6935415821 | 1.0595431684 |
| C12 | -4.9932865389 | -2.6327170642 | 2.0486467238 |
| H13 | -5.8460362440 | -2.6811749753 | 2.7413791094 |
| C14 | -5.8033360479 | -4.6950611258 | 1.0099553249 |
| H15 | -6.6327333649 | -4.7470320708 | 1.7108038818 |
| H16 | -5.7327515406 | -5.4889096728 | 0.2743380871 |
| H17 | -4.0789848521 | -3.6454717965 | 0.3567583719 |
| O18 | 0.4981888781 | -0.9906926285 | 4.5013194087 |

| | | | |
|---|---|---|---|
| O19 | -1.0815350599 | -2.1190446181 | 2.0808231940 |
| H20 | -1.6893557331 | 2.1791184933 | -1.1358800934 |
| H21 | -2.0261971536 | -2.1971419940 | 1.8267785253 |

**7** (another isomer)
Energy = -977.340957
Zero Point Energy (ZPE): 69.163 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.7624029083 | 0.2034510120 | -0.5061752546 |
| O2 | 2.3742968277 | -0.7297268901 | -0.0879085627 |
| O3 | 1.1430536653 | 1.8593316435 | -0.5252073288 |
| O4 | -0.2860587280 | -0.1671764240 | 1.0461290903 |
| O5 | -0.0392474764 | -0.7217366784 | -1.9825047407 |
| Mo6 | 0.0469968548 | -1.0054221831 | 2.7605121724 |
| O7 | 1.8498629043 | -1.5582716175 | 2.4985562552 |
| Mo8 | 3.2104972941 | -1.8463740669 | 1.2132800501 |
| O9 | -0.0117698881 | 0.0763558907 | 4.0722797430 |
| N10 | -1.0007067255 | -2.5678069504 | 2.9778497524 |
| C11 | -1.0190081956 | -4.0806797317 | 4.8781963894 |
| C12 | -1.5648828511 | -3.4922701407 | 3.6626180947 |
| H13 | -2.5279521538 | -3.8892064262 | 3.3126509322 |
| C14 | -1.6627594806 | -5.0457977270 | 5.5554154920 |
| H15 | -2.6248697954 | -5.4279880570 | 5.2236531104 |
| H16 | -1.2496350590 | -5.4769930135 | 6.4612540831 |
| H17 | -0.0586974171 | -3.6978341292 | 5.2164647146 |
| O18 | 4.6462320596 | -1.1431084287 | 1.7833047038 |
| O19 | 3.2332160246 | -3.6720645340 | 0.6544840362 |
| H20 | -0.2946499569 | -0.2642626472 | -2.7960091898 |
| H21 | 2.4371945323 | -4.1708302010 | 0.4181083353 |

**TS5**
Energy = -977.285664
Zero Point Energy (ZPE): 67.721 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.5788046938 | 0.4684278611 | -0.0688473301 |
| O2 | 2.3586673365 | -0.0950343098 | -0.0931310908 |
| O3 | 0.1436967986 | 1.9300207966 | -0.8208085810 |
| O4 | -0.1546994237 | 0.1080969969 | 1.6841403310 |
| O5 | -0.0799038934 | -1.0495811754 | -1.1320943797 |
| Mo6 | 0.3019958482 | -1.3936387782 | 2.7915955010 |
| O7 | 2.1479194159 | -1.5272599744 | 2.4093717275 |
| Mo8 | 3.1098388879 | -1.7476318641 | 0.7230382074 |
| O9 | 0.0266759068 | -1.4437590739 | 4.4705261831 |

| | | | |
|---|---|---|---|
| N10 | -0.3806767312 | -2.9379950150 | 1.9540501901 |
| C11 | -1.5013616189 | -4.2264551378 | 0.2737968449 |
| C12 | -0.3160947198 | -3.7246390076 | 0.9679098459 |
| H13 | 1.0217469022 | -3.5560726568 | 0.2280686090 |
| C14 | -1.3751200368 | -5.0147979569 | -0.8061128787 |
| H15 | -0.3957402624 | -5.2959925818 | -1.1831139152 |
| H16 | -2.2420667047 | -5.3987510806 | -1.3350602796 |
| H17 | -2.4841166439 | -3.9548433197 | 0.6602067409 |
| O18 | 4.7883122551 | -1.9967551597 | 0.6831601078 |
| O19 | 1.7807237229 | -2.9966379895 | -0.3700016414 |
| H20 | 1.2113495560 | -2.4329140081 | -0.9467984090 |
| H21 | -1.0288190804 | -1.2344913898 | -1.0702544194 |

**6** (no Mo-Mo bonds)
Energy = -806.430563 hartrees
Zero Point Energy (ZPE): 36.856 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 2.0012324540 |
| O3 | 1.5569707401 | 0.0000000000 | -0.6661710987 |
| O4 | -1.3755442833 | 1.2789112306 | -0.3959745093 |
| O5 | -0.8688737830 | -1.9601935028 | 0.2904197729 |
| Mo6 | -2.7832619713 | 1.9658072542 | 0.7323132592 |
| O7 | -2.5752380070 | 1.3387715645 | 2.5169786077 |
| Mo8 | -1.4294111157 | -0.0750140854 | 3.1798482263 |
| O9 | -3.9186413008 | 3.1393554789 | 0.2720289167 |
| O10 | -1.2455997456 | -0.2037804941 | 4.8695689700 |
| O11 | -2.3179365208 | -1.6854386359 | 2.3771411941 |
| H12 | -1.2960072652 | -2.4070334876 | -0.4513153121 |
| H13 | -1.4764128732 | -2.0054713349 | 1.1129906796 |
| H14 | -3.2840620242 | -1.6811737254 | 2.3337312088 |

**6** (one Mo-Mo bond)
Energy = -806.448963 hartrees
Zero Point Energy (ZPE): 37.693 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9433024693 |
| O3 | 1.5250321062 | 0.0000000000 | -0.7397551360 |
| O4 | -1.5745061426 | 0.6408361354 | -0.9766840054 |
| O5 | -1.2115027671 | -1.8432951398 | 0.2531894654 |
| Mo6 | -1.4756949302 | 2.3082263696 | -0.0371006883 |
| O7 | -2.0358861064 | 2.1453025846 | 1.8466491032 |
| Mo8 | -1.4813668742 | 0.6769904323 | 2.9142794746 |
| O9 | -0.6293556663 | 3.6199920315 | -0.7015199256 |
| O10 | -1.0584753832 | 0.8376275727 | 4.5534396364 |

| | | | |
|---|---|---|---|
| O11 | -2.4545550060 | -0.9847980859 | 2.4109569330 |
| H12 | -1.8729446671 | -1.8941366845 | -0.4542337059 |
| H13 | -1.7236820113 | -1.7128551168 | 1.1089614817 |
| H14 | -3.3097957097 | -1.1643925493 | 2.8241017696 |

**6** (two Mo-Mo bonds)
Energy = -806.464285 hartrees
Zero Point Energy (ZPE): 37.429 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.0056319701 | 0.1872804517 | 1.1579567388 |
| O2 | -1.6472137027 | 1.5453062308 | 1.6205613045 |
| O3 | -4.6098767645 | 0.6164776185 | 0.8080964013 |
| O4 | -2.5905102329 | -1.5785017702 | 1.8980251387 |
| O5 | -1.5324645001 | -0.4839951117 | -0.4197005538 |
| Mo6 | -2.6483437032 | -0.7199611837 | 3.6272425957 |
| O7 | -0.9498249466 | -0.1502088470 | 4.4016819663 |
| Mo8 | -0.9742722646 | 1.4611613240 | 3.3997854898 |
| O9 | -4.0753253476 | -0.4200922334 | 4.4987764196 |
| H10 | -0.7385273026 | 0.0741249452 | -0.4049782384 |
| H11 | 1.4624731881 | 2.1796380004 | 3.3945258722 |
| O12 | 0.9127895812 | 1.4682486118 | 3.0344977238 |
| O13 | -1.6489522587 | 2.6739178089 | 4.3756662621 |
| H14 | -1.2608691471 | -1.3834452502 | -0.1711773492 |

**Acrylonitrile ($NCCHCH_2$)**
Energy = -170.831737 h
Zero Point Energy (ZPE): 31.919 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| N10 | -1.8901790706 | -2.9628423705 | 3.4886842466 |
| C12 | -0.8242528072 | -5.3153734415 | 3.2448360668 |
| C13 | -1.4231056686 | -4.0233819979 | 3.3856505277 |
| C16 | -1.3936193272 | -6.4369089061 | 3.7027574526 |
| H17 | -2.3519768630 | -6.4256238058 | 4.2110799068 |
| H18 | -0.9042300694 | -7.3966281959 | 3.5753914118 |
| H19 | 0.1369253160 | -5.3379205277 | 2.7374303011 |

Desorption of $H_2O$ from **5**
Energy = -900.831389
Zero Point Energy (ZPE): 53.651 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.2711318342 | 1.5884645047 | 1.4952201880 |
| O2 | -1.4600676638 | 1.9302316427 | 2.1003750198 |
| O3 | -4.2564279415 | 2.7712018888 | 0.7648081654 |

| | | | |
|---|---|---|---|
| O4 | -3.9242905017 | 0.0819682014 | 2.4330581088 |
| Mo6 | -3.1174256421 | -1.1324149678 | 3.7341745834 |
| O7 | -1.4037218695 | -0.2592559629 | 3.9124643198 |
| Mo8 | -0.1711365393 | 0.8337886791 | 2.9758633477 |
| O9 | -4.0298572733 | -1.5962515527 | 5.0944749232 |
| N10 | -3.0067611024 | -2.8109851503 | 2.5605684190 |
| C11 | -3.2383991690 | -5.0723224957 | 1.3326452938 |
| C12 | -3.1105608397 | -3.8391663417 | 2.0081974103 |
| C13 | -3.7354288989 | -6.1813651629 | 1.9136581811 |
| H14 | -4.0586602958 | -6.1932753144 | 2.9488894927 |
| H15 | -3.8304811971 | -7.0991000117 | 1.3450084784 |
| H16 | -2.9211167471 | -5.0664895392 | 0.2926639785 |
| O17 | 0.7090527336 | 1.7393293858 | 4.1140820744 |
| O18 | 0.6674313946 | -0.2630272654 | 1.6436207686 |
| H21 | 1.6288822847 | -0.2913963046 | 1.5386161379 |

Desorption of $H_2O$ from **5** (one Mo-Mo bond)
Energy = -900.86159246938 hartrees
Zero Point Energy (ZPE): 53.646 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| C1 | -1.4675343164 | -6.3701995364 | 3.6956240651 |
| C2 | -0.7154271649 | -5.2876782889 | 3.4394905641 |
| C3 | -1.2600172126 | -3.9762009564 | 3.4033962973 |
| N4 | -1.6885467926 | -2.8942801899 | 3.3682486826 |
| Mo5 | -2.7234452477 | -1.0021153090 | 3.6708555887 |
| O6 | -4.0875384581 | -1.1745929108 | 4.6703460739 |
| O7 | -3.0856048303 | -0.6638664411 | 1.7828831822 |
| Mo8 | -2.3844060754 | 0.5568268872 | 0.5311656878 |
| O9 | -0.9211938617 | -0.2574157694 | -0.3967499913 |
| O10 | -1.7539799814 | 1.7693743944 | 1.8793604323 |
| Mo11 | -1.6961163791 | 1.4881758180 | 3.7990001871 |
| O12 | -2.4798491442 | 2.4441243837 | 4.9653711750 |
| O13 | -3.6733581604 | 1.1464335108 | -0.4067646768 |
| O14 | -1.0512711392 | -0.2476905727 | 4.3269986854 |
| H15 | -0.2860748112 | -0.8447479654 | 0.0377754481 |
| H16 | -2.5331446814 | -6.2991780660 | 3.8862766037 |
| H17 | -1.0159821563 | -7.3557688130 | 3.7205366493 |
| H18 | 0.3527915195 | -5.3574841698 | 3.2519031928 |

**8**
Energy = -976.149422 hartrees
Zero Point Energy (ZPE): 57.229 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -0.0665773173 | -0.0816009442 | -0.0698030179 |
| O2 | 1.7286081585 | -0.3727643783 | -0.6723304654 |
| O3 | -0.4087027980 | 1.5711363525 | 0.1652195561 |
| O4 | -0.1554339129 | -1.0382151522 | 1.5754798107 |
| O5 | -1.1868470999 | -0.7092568965 | -1.1958029300 |
| Mo6 | 0.6845949695 | -2.7725609402 | 1.8173156032 |
| O7 | 2.5248583681 | -2.5588790446 | 1.2330896133 |
| Mo8 | 2.9703232423 | -1.8156083530 | -0.4638814583 |
| O9 | 0.3854216818 | -3.6200764823 | 3.2630876012 |
| N10 | -0.0368696750 | -3.7298188086 | 0.3979539767 |
| C11 | -0.9485924376 | -4.9551177925 | -1.4505918697 |
| C12 | -0.6783437785 | -4.7599214093 | -0.0447791235 |
| H13 | -1.0364652656 | -5.5212861852 | 0.6609468882 |
| C14 | -1.6193510498 | -6.0346804987 | -1.8985153504 |
| H15 | -1.9828707958 | -6.7993411374 | -1.2170664401 |
| H16 | -1.8209613387 | -6.1791177302 | -2.9542443802 |
| H17 | -0.5827655222 | -4.1878806763 | -2.1275983906 |
| O18 | 4.5903180635 | -1.2870044321 | -0.4948050243 |
| O19 | 2.7545545296 | -2.9718167716 | -1.7024304626 |

**TS6**

Energy = -976.100424 hartrees

Zero Point Energy (ZPE): 53.852 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.4295524766 | 0.5210633622 | -0.0227092167 |
| O2 | 1.9936817307 | -0.5043665215 | -0.2917010507 |
| O3 | 0.6778544400 | 2.1803449743 | -0.3329784118 |
| O4 | -0.0929991393 | 0.2094610704 | 1.8043223877 |
| O5 | -0.8010555713 | -0.0526455869 | -1.0658291759 |
| Mo6 | 0.4900825115 | -1.3240568789 | 2.8088677582 |
| O7 | 2.3219287894 | -1.3604476011 | 2.3454445011 |
| Mo8 | 2.9532520047 | -1.9532268059 | 0.5933222033 |
| O9 | 0.2327824506 | -1.5173425343 | 4.4765498375 |
| N10 | -0.1995291291 | -2.8139409454 | 1.8922021819 |
| C11 | -1.3443810779 | -4.1704888254 | 0.2448245098 |
| C12 | -0.1960804801 | -3.6853414418 | 0.9904741966 |
| H13 | 1.1867497514 | -3.8350635434 | 0.4779481543 |
| C14 | -1.1773629465 | -5.0749688460 | -0.7341674160 |
| H15 | -0.1931534562 | -5.4620190067 | -0.9808929363 |
| H16 | -2.0195031606 | -5.4432563350 | -1.3112238101 |
| H17 | -2.3269105012 | -3.7731145134 | 0.4931827840 |
| O18 | 4.6490726515 | -1.8509803372 | 0.5806290157 |
| O19 | 2.2202669580 | -3.5530648120 | 0.0868674694 |

**9** (with weak H-bond)

Energy = -976.126246 h
Zero Point Energy (ZPE): 56.171 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.9585922991 | 1.2755005637 | 1.2423098039 |
| O2 | -1.7006440946 | 2.1135784582 | 2.4133735529 |
| O3 | -3.9343044832 | 2.3561570452 | 0.3387942942 |
| O4 | -3.9377803035 | 0.1869177791 | 2.3949195379 |
| O5 | -1.9491504056 | 0.2662159780 | 0.2461287987 |
| Mo6 | -3.1913827133 | -1.0420580534 | 3.7598996950 |
| O7 | -1.4499970354 | -0.2638291196 | 3.9121488445 |
| Mo8 | -0.2747263798 | 1.0399401775 | 3.1451388471 |
| O9 | -4.2002681806 | -1.2992770432 | 5.0982136542 |
| N10 | -3.2677633689 | -2.7322953916 | 2.5694323554 |
| C11 | -3.5461415451 | -4.9225004212 | 1.2285583741 |
| C12 | -3.3968380202 | -3.7236688406 | 1.9643472450 |
| C13 | -4.0767470114 | -6.0366664115 | 1.7639195407 |
| H14 | -4.4038393665 | -6.0792406595 | 2.7973659694 |
| H15 | -4.1989051306 | -6.9280918337 | 1.1594814330 |
| H16 | -3.2214836779 | -4.8770558698 | 0.1921260364 |
| O17 | 0.5667849600 | 1.8111091525 | 4.4003549611 |
| O18 | 0.6647376206 | 0.3803783209 | 1.6418624262 |
| H21 | 0.1011642511 | 0.0668836976 | 0.9056703052 |

**9** (without weak H-bond)
Energy = -976.124069 h
Zero Point Energy (ZPE): 55.981 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.1744599274 | 0.8222561614 | 1.1910387471 |
| O2 | -1.7084123110 | 1.9276464989 | 1.8345659998 |
| O3 | -4.4120966946 | 1.7140376262 | 0.4089176536 |
| O4 | -3.7701068609 | 0.0010118241 | 2.7410770756 |
| O5 | -2.5004675288 | -0.3727212105 | 0.1450356016 |
| Mo6 | -2.7157645182 | -1.1548579279 | 3.9661681336 |
| O7 | -1.1583261282 | -0.0536493730 | 3.9246694955 |
| Mo8 | -0.3386491145 | 1.4685438117 | 3.0675505249 |
| O9 | -3.6063033275 | -1.4407654748 | 5.3746583338 |
| N10 | -3.0889038932 | -2.7604060466 | 2.7178649885 |
| C11 | -3.7891076824 | -4.6652236079 | 1.1210011166 |
| C12 | -3.4033105923 | -3.6235799849 | 1.9976407297 |
| C13 | -4.4851279567 | -5.7389422849 | 1.5333207725 |
| H14 | -4.7722636150 | -5.8758673871 | 2.5704800026 |
| H15 | -4.7885556632 | -6.4988035087 | 0.8223717458 |
| H16 | -3.5065632526 | -4.5206958297 | 0.0812851868 |
| O17 | -0.1739449768 | 2.6379074937 | 4.2870604364 |
| O18 | 1.1891807755 | 0.8552373802 | 2.1008363653 |

| | | | |
|---|---|---|---|
| H21 | 2.0437603732 | 1.3061407939 | 2.1653110405 |

**10** (with one Mo-Mo bond)
Energy = -805.262865
Zero Point Energy (ZPE): 23.661 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5096040099 | 0.0225483490 | 0.8268909762 |
| O2 | -1.6535574990 | 1.5590369714 | 1.6539538549 |
| O3 | -3.9903610145 | 0.5036187853 | 0.1347179189 |
| O4 | -2.7935559122 | -1.3996651330 | 2.0781986807 |
| O5 | -1.5017841764 | -0.5570755774 | -0.4242048894 |
| Mo6 | -2.8389465839 | -0.7146418939 | 3.8835854521 |
| O7 | -1.2341098185 | 0.0309351162 | 4.6612117105 |
| Mo8 | -1.1747797712 | 1.5276941705 | 3.4911559849 |
| O9 | -4.2875305790 | -0.2543968654 | 4.6208169036 |
| H10 | 1.2147896498 | 2.3836711263 | 3.6118000510 |
| O11 | 0.7232266663 | 1.5749272934 | 3.4021812090 |
| O12 | -1.9536838677 | 2.8089367658 | 4.2688396465 |

**10** (with no Mo-Mo bond)
Energy = -805.246119 hartrees
Zero Point Energy (ZPE): 22.893 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.0127388041 | 1.1831636766 | 1.0861974729 |
| O2 | -1.4150475287 | 1.6701348139 | 2.0078177325 |
| O3 | -4.0067071964 | 2.5446260045 | 0.8220922766 |
| O4 | -3.8848780362 | -0.1343846359 | 2.1612925206 |
| O5 | -2.6122404120 | 0.5029869345 | -0.4297983803 |
| Mo6 | -3.2194311504 | -0.8534586778 | 3.8194006387 |
| O7 | -1.4193412124 | -0.2382134472 | 4.0288851780 |
| Mo8 | -0.1344840155 | 0.9193862924 | 3.2248927653 |
| O9 | -4.2019252276 | -1.1230749335 | 5.1679881261 |
| O10 | 0.3459718096 | 2.0339451677 | 4.4055268011 |
| O11 | 1.1402533491 | -0.1134890722 | 2.2656974460 |
| H12 | 2.0982529877 | 0.0049970323 | 2.3534795736 |

## Allylic O-insertion

**1-π-allyl**
Energy = -977.309977 hartrees
Zero Point Energy (ZPE): 68.354 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0287028672 | -0.0048350274 | -0.0241599938 |

| | | | |
|---|---|---|---|
| O2 | 0.0240949486 | 0.0127131962 | 1.8895691617 |
| O3 | 1.6167605187 | 0.0116411523 | -0.6431231106 |
| O4 | -0.9730761642 | 1.5168367703 | -0.5721220390 |
| O5 | -0.7189343665 | -1.4225883764 | -0.5993097756 |
| Mo6 | -1.9496347142 | 2.8808690787 | 0.3803373664 |
| O7 | -1.5164070732 | 2.6201569154 | 2.2431710179 |
| Mo8 | -1.0719963406 | 0.9868739794 | 3.1194974845 |
| N9 | -1.4289762252 | 4.4836738597 | -0.1142005123 |
| O10 | -3.6185648806 | 2.7426028850 | 0.0966807174 |
| O11 | -0.3557582757 | 1.2176573126 | 4.6474558119 |
| O12 | -2.5127295737 | 0.1057080992 | 3.3551592337 |
| C13 | 2.3237889879 | 2.5895178282 | 1.8957790655 |
| C14 | 1.8932192965 | 3.0483425714 | 3.1334376236 |
| H15 | 2.1740528591 | 2.5492074708 | 4.0537549148 |
| H16 | 1.2820228621 | 3.9427148491 | 3.2179450457 |
| C17 | 2.0260339372 | 3.1899253070 | 0.6798940475 |
| H18 | 1.4313645856 | 4.0981276443 | 0.6317566383 |
| H19 | 2.4071632066 | 2.7890300213 | -0.2527709025 |
| H20 | 2.9427590439 | 1.6930143339 | 1.8757317771 |
| H21 | -1.8853802138 | 5.3011531615 | -0.5240122414 |

**TS-oxo**

Energy = -977.302978 hartrees

Zero Point Energy (ZPE): 68.669 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1464782899 | -0.0007194013 | 0.1778225578 |
| O2 | 1.5775595715 | -1.2837413716 | -0.0222366534 |
| O3 | 0.6232722004 | 1.4919652261 | -0.4908898045 |
| O4 | 0.0349814554 | 0.0272595763 | 2.1020290054 |
| O5 | -1.3213427246 | -0.5753905955 | -0.5827799878 |
| Mo6 | 0.8175323238 | -0.9026204909 | 3.5757438670 |
| O7 | 2.2594879915 | -1.9370419806 | 2.8180625694 |
| Mo8 | 2.5094991633 | -2.5470772233 | 1.0303960033 |
| O9 | 1.3639681697 | 0.1520988921 | 4.7983533097 |
| N10 | -0.3834065532 | -2.0037696488 | 4.2516125601 |
| H11 | -0.7750608467 | -2.1614584358 | 5.1804992256 |
| C12 | -1.4007357883 | -3.4616409948 | -1.1105592458 |
| C13 | -1.1239042636 | -4.2636524146 | -0.0380414062 |
| H14 | -0.3783595308 | -5.0485604350 | -0.0863838103 |
| H15 | -1.6365755681 | -4.1268719068 | 0.9110545461 |
| C16 | -2.3479122342 | -2.4172678190 | -1.0681498014 |
| H17 | -2.9776207287 | -2.2822159441 | -0.1963779890 |
| H18 | -2.6592873439 | -1.9138964153 | -1.9744481473 |
| H19 | -0.8601947044 | -3.6217050517 | -2.0414323492 |
| O20 | 1.8091644831 | -4.1029565636 | 0.8331661493 |

| | | | |
|---|---|---|---|
| O21 | 4.1600946374 | -2.6342442144 | 0.6045281726 |

**2-oxo**
Energy = -977.341121 hartrees
Zero Point Energy (ZPE): 70.986 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -0.0165058591 | 0.1878527054 | 0.0801323695 |
| O2 | 1.7470768009 | -0.6055919026 | 0.0031126936 |
| O3 | 0.1564688270 | 1.8391711891 | 0.4207944381 |
| O4 | -0.5413019264 | -0.7666230319 | 1.6678070580 |
| O5 | -1.1415107639 | -0.2402150291 | -1.3578207228 |
| Mo6 | 0.3483029993 | -1.4955911136 | 3.1947790620 |
| O7 | 1.9876888981 | -2.2469619337 | 2.5117054076 |
| Mo8 | 2.8107524916 | -1.9379395688 | 0.8243530849 |
| O9 | 0.6635114400 | -0.3081993571 | 4.3750718581 |
| N10 | -0.6577221831 | -2.7658099974 | 3.8854369763 |
| H11 | -1.0435798535 | -2.9494417716 | 4.8131884135 |
| C12 | -0.4464869201 | -2.5180605066 | -1.8980597484 |
| C13 | -0.5151530924 | -3.6510437755 | -1.1951262195 |
| H14 | 0.3142354468 | -4.3507835215 | -1.1736719140 |
| H15 | -1.4005191596 | -3.9145822550 | -0.6206053818 |
| C16 | -1.5460380420 | -1.4991628245 | -1.9503916906 |
| H17 | -2.4369307127 | -1.8438029669 | -1.4134439513 |
| H18 | -1.8296391866 | -1.2574797112 | -2.9811295527 |
| H19 | 0.4507945399 | -2.2818992455 | -2.4687385405 |
| O20 | 2.8135277832 | -3.3657500963 | -0.1211360915 |
| O21 | 4.4244651029 | -1.4111501243 | 1.0069241172 |

## Ammoxidation of allyl on $Mo3O_7(NH)_2$ – Figure 7

**11**
Energy = -840.145624 hartrees
Zero Point Energy (ZPE): 32.680 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7362931334 | 0.5796876004 | 0.8329886893 |
| O2 | -0.9573460778 | 0.6714012443 | 1.5049654908 |
| O3 | -3.4732045074 | 2.1182980013 | 0.8815695444 |
| O4 | -3.6113313691 | -0.6170537294 | 2.0273511037 |
| O5 | -2.7817318257 | 0.0204041805 | -0.7762799320 |
| Mo6 | -3.3880574525 | -0.8734858352 | 3.9272793260 |
| O7 | -1.5151218970 | -0.5658914756 | 4.2076763178 |

| | | | |
|---|---|---|---|
| Mo8 | -0.3003298748 | 0.6240337243 | 3.3191003623 |
| O9 | -3.8871361848 | -2.4115706327 | 4.4523521921 |
| N10 | -0.4472808699 | 2.2299285821 | 4.0145851793 |
| O11 | 1.3169970294 | 0.1110009839 | 3.4265855811 |
| N12 | -4.3118817846 | 0.3568268486 | 4.7740019723 |
| H13 | -5.0560045614 | 0.4075877745 | 5.4708660145 |
| H14 | 0.1540274683 | 2.9315367615 | 4.4482721898 |

**12**

Energy = -957.471519 h

Zero Point Energy (ZPE): 78.796 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.8773781389 | 1.1074013644 | 0.8159773255 |
| O2 | -1.7677710975 | 2.0987805461 | 2.0533452191 |
| O3 | -4.4715154686 | 1.7105556706 | 0.8050052507 |
| O4 | -2.7658548333 | -0.6868482060 | 1.4483927091 |
| N5 | -2.1974948439 | 1.1874028602 | -0.8081419500 |
| Mo6 | -2.8320119821 | -1.5728381068 | 3.1755561293 |
| O7 | -2.1229394737 | -0.0339378498 | 4.1503232706 |
| Mo8 | -0.9405189880 | 1.3201547051 | 3.5782906520 |
| O9 | -4.4068867631 | -1.9217089664 | 3.7011075530 |
| N10 | -1.5548383043 | -3.0143940981 | 3.2286537515 |
| H11 | -1.8563446231 | -3.9320179228 | 3.5579551937 |
| C12 | 0.6629616672 | -3.2902210149 | 4.2557205222 |
| C13 | -0.0959858350 | -2.9619582360 | 2.9960542426 |
| H14 | 0.1598656694 | -1.9532416670 | 2.6509695292 |
| H15 | 0.1611028396 | -3.6656487954 | 2.1942322083 |
| C16 | 1.4641123453 | -4.3477986894 | 4.3889992335 |
| H17 | 1.6272474367 | -5.0503188497 | 3.5748036673 |
| H18 | 2.0003474465 | -4.5400875358 | 5.3134219984 |
| H19 | 0.5212871704 | -2.5983438652 | 5.0847251697 |
| O20 | 0.5331905277 | 0.5683419391 | 3.1129540600 |
| O21 | -0.6340922125 | 2.4592619065 | 4.8138795937 |
| H22 | -2.5331611904 | 1.5468295964 | -1.7033052376 |

**TS7**

Energy = -957.430627 h

Zero Point Energy (ZPE): 75.959 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.2385465750 | 0.4264514346 | 0.1144608099 |
| O2 | -0.0754208987 | -0.1431359070 | 1.9095984713 |
| O3 | 1.8755085901 | 0.6096413123 | -0.3147396027 |
| O4 | -0.7194966172 | 2.0280940165 | 0.0610436156 |

| | | | |
|---|---|---|---|
| N5 | -0.6566050616 | -0.7639676395 | -0.9970527040 |
| Mo6 | -2.6865654811 | 2.1199751067 | -0.0856073888 |
| H7 | -1.8657812888 | -0.6672512699 | -1.3298324235 |
| C8 | -3.2697043799 | -0.4981765770 | -1.5051414003 |
| O9 | -3.1538394427 | 3.7239230707 | -0.3778383664 |
| N10 | -3.5138183980 | 0.8688571218 | -1.3507528382 |
| C11 | -3.6799121575 | -1.1687791114 | -2.7468698815 |
| Mo12 | -1.7605532766 | 0.1454525991 | 2.8098033574 |
| H13 | -3.4532947941 | -1.0538315698 | -0.5794614583 |
| O14 | -2.8485306834 | 1.0508040287 | 1.5765434008 |
| C15 | -3.8287109842 | -0.5972824575 | -3.9525154263 |
| H16 | -3.6409833060 | 0.4593062432 | -4.1316451161 |
| H17 | -4.1367424201 | -1.1792015221 | -4.8140550292 |
| H18 | -3.8377293742 | -2.2415836254 | -2.6493228484 |
| O19 | -1.5368817210 | 1.0533031446 | 4.2393749228 |
| O20 | -2.4730948120 | -1.3545051804 | 3.2243466831 |
| H21 | -0.2021671778 | -1.3467921561 | -1.7018223251 |
| H22 | -4.0130616678 | 1.2838527264 | -2.1405593093 |

**13**

Energy = -957.478896 h

Zero Point Energy (ZPE): 79.200 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6653843272 | 0.7278881817 | 0.6613716383 |
| O2 | -2.1383775373 | 1.8968366923 | 2.1198375422 |
| O3 | -3.9718985575 | 1.2899062857 | -0.2647885722 |
| O4 | -3.2542331565 | -0.5909732779 | 1.8910955250 |
| N5 | -1.0291888308 | 0.2423530188 | -0.2663955089 |
| Mo6 | -3.1310384001 | -1.2530153959 | 3.6714654225 |
| O7 | -2.0012525254 | 0.1243998521 | 4.5112549911 |
| Mo8 | -0.9826366682 | 1.3598035926 | 3.5179917179 |
| O9 | -4.5542123555 | -1.6463359592 | 4.5160699738 |
| N10 | -1.6463811220 | -2.7551211490 | 3.7200020716 |
| H11 | -1.9472298071 | -3.7021531360 | 3.9555853934 |
| C12 | 0.5909713428 | -3.7142284900 | 3.6487586518 |
| C13 | -0.3586520242 | -2.6328287959 | 3.5402122120 |
| H14 | -0.1874848189 | -0.0738371167 | 0.2103721054 |
| H15 | 0.0196366648 | -1.6406752360 | 3.2854180583 |
| C16 | 1.9090882297 | -3.5083829931 | 3.4705656585 |
| H17 | 2.2972732573 | -2.5215903562 | 3.2327488520 |
| H18 | 2.6284329347 | -4.3148718312 | 3.5641557295 |
| H19 | 0.2114302182 | -4.7060538731 | 3.8923179944 |
| O20 | 0.2852166217 | 0.4273259422 | 2.7591802682 |
| O21 | -0.3980454877 | 2.6602752861 | 4.4717498943 |
| H22 | -0.8844430408 | 0.3436534113 | -1.2667906682 |

**13** (another isomer)
Energy = -957.480511 hartrees
Zero Point Energy (ZPE): 78.988 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.5349215293 | 0.2278538724 | -0.2406145865 |
| O2 | 2.3754940349 | -0.3552754532 | -0.1440663135 |
| O3 | 0.2165164028 | 1.6442368288 | -1.1376831310 |
| O4 | -0.1165200011 | 0.1130351579 | 1.5524712469 |
| N5 | -0.1510646602 | -1.3253246274 | -1.2026321992 |
| Mo6 | 0.4856009799 | -0.9824750348 | 3.0371372949 |
| O7 | 2.3884377097 | -1.2866606221 | 2.5974136117 |
| Mo8 | 3.0046634609 | -1.8181956447 | 0.9024040697 |
| O9 | -0.0618479826 | -0.7812069534 | 4.6327611249 |
| N10 | -0.0114855351 | -2.9511780915 | 2.5949279954 |
| C11 | -1.3613143160 | -3.7863197879 | 4.4382414884 |
| C12 | -0.6668676838 | -3.9122839474 | 3.1788362102 |
| H13 | -0.6888380402 | -4.8832596095 | 2.6815892549 |
| C14 | -2.0140283063 | -4.8262761990 | 4.9859707503 |
| H15 | -2.0421556249 | -5.8008547934 | 4.5052185438 |
| H16 | -2.5366375232 | -4.7312508002 | 5.9315505069 |
| H17 | -1.3332064146 | -2.8188353748 | 4.9322064866 |
| O18 | 4.6950978050 | -2.0872920852 | 0.8292816418 |
| O19 | 2.0699347309 | -3.2258101724 | 0.4826342864 |
| H20 | 0.4529754559 | -3.2415319063 | 1.7221904466 |
| H21 | 0.4740401862 | -1.9865914631 | -1.6563104408 |
| H22 | -1.0827324710 | -1.3526847131 | -1.6042472594 |

**TS8**
Energy = -957.467452 h
Zero Point Energy (ZPE): 76.873 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1363528459 | 0.0207546053 | 0.1275587231 |
| O2 | -0.1464499614 | -0.0923746528 | 2.0720615584 |
| O3 | 1.6692070826 | 0.1663936363 | -0.6018737814 |
| O4 | -1.2940619404 | 1.2686842282 | -0.2836476645 |
| N5 | -1.0023047654 | -1.6898461878 | -0.4242756815 |
| Mo6 | -3.0846518019 | 1.1576641075 | 0.3504140522 |
| O7 | -2.9883120147 | 0.6821621085 | 2.2190219122 |
| Mo8 | -1.7371486588 | -0.5758812151 | 2.9589770822 |
| O9 | -4.3179588634 | 2.1677244128 | -0.2398118008 |
| N10 | -3.3746496459 | -0.6257824265 | -0.5553132361 |
| H11 | -2.2826982700 | -1.2555870969 | -0.5031617953 |

| | | | |
|---|---|---|---|
| C12 | -4.4222697037 | -2.4496382070 | -1.7519350228 |
| C13 | -4.3795383124 | -1.1024393397 | -1.2114846425 |
| H14 | -0.9717739413 | -2.4374657506 | 0.2727059504 |
| H15 | -5.2585406342 | -0.4718780270 | -1.3802068500 |
| C16 | -5.4872042926 | -2.9087540092 | -2.4292582243 |
| H17 | -6.3599063042 | -2.2844600463 | -2.6027868462 |
| H18 | -5.5196091938 | -3.9187448167 | -2.8232036352 |
| H19 | -3.5582838971 | -3.0860648976 | -1.5748804363 |
| O20 | -2.1762296563 | -2.1583135718 | 2.4249901338 |
| O21 | -1.6161840902 | -0.4988907780 | 4.6644199499 |
| H22 | -0.7127909352 | -2.0805646690 | -1.3214125997 |

**14**
Energy = -957.476830 h
Zero Point Energy (ZPE): 79.804 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.9170861298 | 0.6040071488 | 0.7324997849 |
| O2 | -2.2653631849 | 1.9692419177 | 2.0385852202 |
| O3 | -3.8533909137 | 1.0145028692 | -0.6253408571 |
| O4 | -3.5729921492 | -0.7115234846 | 2.0384798257 |
| N5 | -0.9276993858 | -0.4739863305 | 0.5827992241 |
| Mo6 | -2.8431139511 | -1.2510421938 | 3.6931443499 |
| O7 | -1.9501949901 | 0.3006525374 | 4.4422910821 |
| Mo8 | -1.0773910712 | 1.6759919418 | 3.4491587938 |
| O9 | -3.7918387787 | -2.2386546709 | 4.7073433535 |
| N10 | -1.4221225158 | -2.3888421658 | 3.0710276604 |
| H11 | -0.9603361867 | -1.3067886324 | 1.1890287059 |
| C12 | 0.1283693787 | -4.2295661811 | 2.8583509336 |
| C13 | -1.0856158936 | -3.6033534332 | 3.3516255977 |
| H14 | -0.1738663971 | 0.1062028696 | 0.9732110108 |
| H15 | -1.7264367082 | -4.2179647742 | 4.0009725842 |
| C16 | 0.4561927023 | -5.4965182757 | 3.1666699791 |
| H17 | -0.1840907418 | -6.1078563813 | 3.7975750848 |
| H18 | 1.3694767735 | -5.9551941458 | 2.8032522639 |
| H19 | 0.7765283219 | -3.6184635945 | 2.2339319578 |
| O20 | 0.3670247131 | 1.0257229496 | 2.7387136402 |
| O21 | -0.7413087394 | 3.0786138152 | 4.3696277108 |
| H22 | -0.6713618163 | -0.7653720645 | -0.3591744087 |

**14** (another isomer)
Energy = -957.481753 h
Zero Point Energy (ZPE): 79.803 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.6125637036 | 0.2942215370 | -0.2046598497 |

| | | | |
|---|---|---|---|
| O2 | 2.4970279630 | -0.3223462410 | -0.0438192292 |
| O3 | 0.0526217278 | 1.3080112855 | -1.4459446195 |
| O4 | 0.0331696988 | 0.3182378722 | 1.6817735992 |
| N5 | -0.1508512883 | -1.7420780744 | -0.6236756608 |
| Mo6 | 0.4128891829 | -0.9984322100 | 2.9920840703 |
| O7 | 2.2479318509 | -1.4970342668 | 2.6361278005 |
| Mo8 | 3.0432113514 | -1.8316166979 | 0.9342435489 |
| O9 | 0.0443440405 | -0.7075559823 | 4.6347389472 |
| N10 | -0.5232519361 | -2.5692577399 | 2.4039032861 |
| C11 | -1.2378575660 | -3.8797183056 | 4.3439768788 |
| C12 | -1.1245534034 | -3.5876333982 | 2.9248627484 |
| H13 | -1.5869268816 | -4.3138429843 | 2.2431241504 |
| C14 | -1.8509560267 | -4.9871647978 | 4.7977763140 |
| H15 | -2.2934396327 | -5.7121377706 | 4.1186790712 |
| H16 | -1.9243539979 | -5.2009784238 | 5.8592917682 |
| H17 | -0.7993298186 | -3.1605437763 | 5.0326724933 |
| O18 | 4.7448539850 | -2.0226948536 | 0.9852568578 |
| O19 | 2.2685204754 | -3.2050927785 | 0.2157738816 |
| H20 | 0.5922736682 | -2.3815538708 | -0.9210871936 |
| H21 | -0.8902137008 | -1.7366203541 | -1.3253468651 |
| H22 | -0.5260798813 | -2.1420936495 | 0.2500399550 |

**TS9**

Energy = -957.424679 h

Zero Point Energy (ZPE): 76.945 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.5062977317 | 0.5805743999 | 0.0006882548 |
| O2 | 2.3564470417 | -0.2062098962 | -0.1987944796 |
| O3 | 0.2465971647 | 2.1123945459 | -0.6854351349 |
| O4 | -0.0603607678 | 0.0278134334 | 1.7205893421 |
| N5 | 0.0832175580 | -0.9474185288 | -1.5768139356 |
| Mo6 | 0.3949263196 | -1.4818566825 | 2.8940061466 |
| O7 | 2.3289240071 | -1.4934344112 | 2.3351242590 |
| Mo8 | 2.9312625340 | -1.7515167631 | 0.6087713489 |
| O9 | 0.2719046224 | -1.4909429218 | 4.5911583204 |
| N10 | -0.3053437787 | -3.0139049832 | 1.9879744461 |
| C11 | -1.4399305173 | -4.3208283179 | 0.3025855413 |
| C12 | -0.2782897055 | -3.8271823397 | 1.0407038902 |
| H13 | 1.1684681744 | -3.6495830788 | 0.2987007269 |
| C14 | -1.2843353252 | -5.1069643651 | -0.7739322256 |
| H15 | -0.2951537038 | -5.4047541155 | -1.1105468349 |
| H16 | -2.1371221530 | -5.4737022437 | -1.3376861354 |
| H17 | -2.4333990136 | -4.0331367826 | 0.6498833760 |
| O18 | 4.6197141232 | -1.9614920639 | 0.4760498553 |
| O19 | 1.9083049466 | -3.1032222072 | -0.2323814030 |
| H20 | 0.5577992826 | -1.8209184547 | -1.3091948760 |

| | | | |
|---|---|---|---|
| H21 | -0.8958862772 | -1.1532822064 | -1.7626966983 |
| H22 | 0.5117749198 | -0.6458467901 | -2.4523614374 |

**15**
Energy = -957.451831
Zero Point Energy (ZPE): 78.134 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7473160813 | 0.6652080154 | 0.7669125768 |
| O2 | -1.9824583306 | 1.8920491170 | 2.0208081964 |
| O3 | -3.6786743326 | 1.3334427181 | -0.4982137174 |
| O4 | -3.3448012374 | -0.7299572029 | 1.8400564853 |
| N5 | -0.6687576779 | 0.4567061457 | 0.0282260801 |
| Mo6 | -3.1385959677 | -1.2651497777 | 3.7440416799 |
| O7 | -2.1746554488 | 0.2189742508 | 4.4115522850 |
| Mo8 | -0.9457312897 | 1.4989156253 | 3.5948611081 |
| O9 | -4.5350841819 | -1.9166220811 | 4.4705144676 |
| N10 | -1.9302873952 | -2.8847839959 | 3.4315499299 |
| H11 | -0.1070248562 | 0.2353628792 | 0.8782571004 |
| C12 | -0.6716573391 | -5.1407348486 | 3.3991469719 |
| C13 | -1.3660313239 | -3.9136476259 | 3.4008029944 |
| H14 | -0.3348943128 | 1.3568569056 | -0.3156672517 |
| C15 | -1.2031730592 | -6.2980508736 | 3.8417623633 |
| H16 | -2.2120328844 | -6.3540333755 | 4.2354835609 |
| H17 | -0.6218492758 | -7.2119308499 | 3.8094822806 |
| H18 | 0.3416561052 | -5.0975444361 | 3.0066160572 |
| O19 | 0.3182996449 | 0.2900477318 | 2.6046830638 |
| O20 | -0.2649849404 | 2.7721207798 | 4.5118854798 |
| H21 | -0.5052581368 | -0.2399978075 | -0.6945877955 |
| H22 | 0.8510117017 | -0.3095328099 | 3.1427954589 |

**16** (one Mo-Mo bond)
Energy = -786.598040 hartrees
Zero Point Energy (ZPE): 46.285 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -0.0156871542 | -0.0176960747 | -0.0018651881 |
| O2 | 1.8986356060 | -0.0264896850 | 0.0265204560 |
| O3 | -0.7512635375 | 1.5118093005 | -0.0861792647 |
| O4 | -0.9652090302 | -1.5960852824 | 0.6439622075 |

| | | | |
|---|---|---|---|
| N5 | 0.1065781273 | -1.1604227662 | -1.9395520631 |
| Mo6 | -0.0150966611 | -1.4960123875 | 2.3082165685 |
| O7 | 1.8850526365 | -2.0150501521 | 2.1600857929 |
| Mo8 | 2.9269639649 | -1.4474851833 | 0.6768792481 |
| O9 | -0.7087608143 | -0.6719294248 | 3.6190097126 |
| O10 | 4.5405877422 | -0.9400495638 | 0.8616351239 |
| O11 | 2.4764289467 | -2.5463576316 | -0.9050733162 |
| H12 | -0.7481287030 | -1.6793628730 | -2.1336372732 |
| H13 | 0.8828914610 | -1.8258882281 | -1.8076554474 |
| H14 | 2.9401104502 | -3.3915703024 | -0.9876072780 |
| H15 | 0.3276344942 | -0.5756204278 | -2.7430974844 |

**16** (two Mo-Mo bonds)
Energy = -786.615308 hartrees
Zero Point Energy (ZPE): 45.976 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7910740486 | 0.0756759971 | 1.1557719649 |
| O2 | -1.5187573178 | 1.4827137105 | 1.6910716651 |
| O3 | -4.3156172789 | 0.4646482839 | 0.5042852032 |
| O4 | -2.5026656159 | -1.6246387579 | 2.0904036676 |
| N5 | -1.2409987617 | -0.7561440702 | -0.2819396862 |
| Mo6 | -2.7434917003 | -0.6246642485 | 3.7229123449 |
| O7 | -1.1372465528 | -0.0146798027 | 4.6503480434 |
| Mo8 | -1.0094804138 | 1.5091021857 | 3.5271048565 |
| O9 | -4.2610646243 | -0.2291981965 | 4.3799400675 |
| H10 | -1.5432683343 | -0.7745863194 | -1.2545267201 |
| H11 | 1.4424281682 | 2.1530794006 | 3.6979814162 |
| O12 | 0.9044809819 | 1.4369283742 | 3.3306149317 |
| O13 | -1.7407690364 | 2.8084815497 | 4.3389294159 |
| H14 | -0.3798047464 | -0.2126498666 | -0.2273084588 |
| H15 | -1.0404856698 | -1.7116236299 | 0.0139212827 |

**16** (no Mo-Mo bonds)
Energy = -786.578628 hartrees
Zero Point Energy (ZPE): 45.775 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7631805269 | 0.6252689787 | 0.7252813533 |
| O2 | -1.9231636311 | 1.9099336704 | 2.0258002525 |
| O3 | -3.5446952180 | 1.3301267958 | -0.6074269518 |

| | | | |
|---|---|---|---|
| O4 | -3.3517293792 | -0.8243452343 | 1.8385703715 |
| N5 | -0.6537997406 | 0.3804512005 | 0.1092123928 |
| Mo6 | -3.2774821740 | -1.0849596538 | 3.7607182250 |
| O7 | -1.9743353468 | 0.1208495573 | 4.4654233352 |
| Mo8 | -0.9494901526 | 1.4836340667 | 3.5512867882 |
| O9 | -4.0706375669 | -2.2772291490 | 4.6800577622 |
| H11 | -0.1230185423 | 0.1381393551 | 0.9687374481 |
| H14 | -0.2823086920 | 1.2756146025 | -0.2099637256 |
| O19 | 0.3593608562 | 0.2191890438 | 2.7709960865 |
| O20 | -0.2075515125 | 2.6705429027 | 4.5268171048 |
| H21 | -0.4674481533 | -0.3133215631 | -0.6113858293 |
| H22 | 0.5169181765 | -0.5805162801 | 3.2944975201 |

**TS10**

Energy = -957.417685 h

Zero Point Energy (ZPE): 74.780 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1635801829 | 0.3531764622 | 0.0785523192 |
| O2 | -0.0783200568 | -0.2405537148 | 1.8526908594 |
| O3 | 1.7750048295 | 0.6274930494 | -0.3972844951 |
| O4 | -0.7811009816 | 1.9538250957 | 0.0937815868 |
| O5 | -0.7204940316 | -0.7827673705 | -1.0485311433 |
| Mo6 | -2.7558861134 | 2.0302093074 | -0.0227532789 |
| H7 | -1.7676391276 | -0.6782184900 | -1.4367485830 |
| C8 | -3.2627522139 | -0.5101759424 | -1.6268170919 |
| O9 | -3.2465698685 | 3.6314764740 | -0.2923615911 |
| N10 | -3.5371345981 | 0.8225941317 | -1.3758532251 |
| C11 | -3.5577823181 | -1.0995865562 | -2.9314818398 |
| Mo12 | -1.6848640254 | 0.2310215185 | 2.8791188135 |
| H13 | -3.3875390670 | -1.1484765800 | -0.7484582676 |
| O14 | -2.9032035614 | 0.9019081182 | 1.5994132697 |
| C15 | -3.6642519212 | -0.4415599208 | -4.0993487402 |
| H16 | -3.5163207783 | 0.6326530888 | -4.1865397692 |
| H17 | -3.8857969181 | -0.9682710557 | -5.0205050603 |
| H18 | -3.6562746176 | -2.1834270409 | -2.9262705877 |
| O19 | -1.3246341915 | 1.3581759481 | 4.1064166008 |
| N20 | -2.3521140316 | -1.2376220363 | 3.5941352251 |
| H21 | -3.9834906254 | 1.2931424544 | -2.1666506835 |
| H22 | -2.5107007335 | -1.5571098154 | 4.5510263678 |

**17**

Energy = -957.455301 h

Zero Point Energy (ZPE): 77.897 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.8679827151 | 0.3795012282 | -0.4344351870 |
| O2 | 2.5231104799 | -0.4875236635 | -0.0966876811 |
| O3 | 0.9910687788 | 2.0730304754 | -0.4943611677 |
| O4 | -0.0418950423 | 0.0084660834 | 1.2315777355 |
| O5 | -0.0610934389 | -0.5574665601 | -1.8227350208 |
| Mo6 | 0.1291358822 | -1.0454334548 | 2.8113338747 |
| O7 | 2.0903063301 | -1.3692868960 | 2.6934425046 |
| Mo8 | 2.9458768173 | -1.9331074300 | 1.1407587190 |
| O9 | -0.4092093753 | -0.5981863328 | 4.3590432940 |
| N10 | -0.1719760488 | -3.0957659708 | 2.6311849504 |
| C11 | -1.1831981450 | -3.8582785366 | 4.7028296465 |
| C12 | -0.6222282491 | -4.0557831987 | 3.3863715226 |
| H13 | -0.5643304318 | -5.0770785013 | 3.0062090184 |
| C14 | -1.6211738586 | -4.8859236664 | 5.4509766679 |
| H15 | -1.5765355509 | -5.9124226738 | 5.0954798202 |
| H16 | -2.0333964071 | -4.7288434489 | 6.4419475899 |
| H17 | -1.2260544273 | -2.8378654868 | 5.0761536636 |
| O18 | 4.6199136960 | -2.2332494849 | 1.3082617734 |
| N19 | 2.0195511213 | -3.3706043763 | 0.5691384737 |
| H20 | -0.2960652977 | -0.1115270116 | -2.6493041303 |
| H21 | 0.2784682271 | -3.4241769235 | 1.7613096076 |
| H22 | 2.3905993443 | -4.2694717394 | 0.2554920318 |

**TS11**

Energy = -957.447912 h

Zero Point Energy (ZPE): 75.894 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5429172217 | 0.5078598582 | 0.6661142813 |
| O2 | -2.1967500669 | 1.9407739473 | 2.0201160793 |
| O3 | -3.5509027786 | 0.8508420921 | -0.6689854756 |
| O4 | -3.3156981309 | -0.6376438563 | 1.9743640042 |
| N5 | -0.7800925432 | -0.0151402779 | 0.3977076531 |
| Mo6 | -3.1495115805 | -1.2115951936 | 3.8040941631 |
| O7 | -2.0149946191 | 0.3029466245 | 4.4960798389 |
| Mo8 | -1.1233518238 | 1.5598218394 | 3.4715993694 |
| O9 | -4.5950695462 | -1.5896303606 | 4.6168274146 |
| N10 | -1.6498587384 | -2.7137261176 | 3.6890751024 |
| H11 | -1.9300975731 | -3.6632795307 | 3.9413590893 |
| C12 | 0.5586747153 | -3.6963951439 | 3.3616736845 |
| C13 | -0.3877664073 | -2.6073092680 | 3.3698085549 |
| H14 | -0.0539167839 | 0.3056425440 | 1.6049279843 |
| H15 | -0.0251906129 | -1.6173871153 | 3.0917557017 |
| C16 | 1.8509999922 | -3.5026265350 | 3.0380317100 |
| H17 | 2.2247585097 | -2.5174918370 | 2.7721602832 |

| | | | |
|---|---|---|---|
| H18 | 2.5645699303 | -4.3195466200 | 3.0336928581 |
| H19 | 0.1964353448 | -4.6884122277 | 3.6289383138 |
| O20 | 0.2580969830 | 0.6807317985 | 2.6054107158 |
| O21 | -0.6647850142 | 2.9312195397 | 4.3751126889 |
| H22 | -0.3115542249 | -0.0817364359 | -0.5075517968 |

**18**

Energy = -957.443428 h

Zero Point Energy (ZPE): 78.389 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -3.1282105424 | 1.2236173543 | 1.2480036699 |
| O2 | -1.7086750824 | 2.0144813876 | 2.2399710970 |
| O3 | -4.1483373565 | 2.3775631341 | 0.5072023652 |
| O4 | -3.8502062247 | -0.0805303992 | 2.3494669958 |
| O5 | -1.8100047149 | 0.3710095919 | 0.0065969505 |
| Mo6 | -3.0150147230 | -1.2129985142 | 3.7714739651 |
| O7 | -1.3729932291 | -0.3057031011 | 3.9244588630 |
| Mo8 | -0.2721392081 | 1.1727966200 | 3.2410125412 |
| O9 | -4.0798385406 | -1.5232596211 | 5.0631982128 |
| N10 | -3.0965771345 | -2.8818195278 | 2.5797223672 |
| C11 | -3.4595315312 | -5.1205143847 | 1.3429773885 |
| C12 | -3.2680070268 | -3.8955514008 | 2.0160862800 |
| C13 | -4.2788949921 | -6.0928944860 | 1.7891547920 |
| H14 | -4.8377430508 | -5.9945016948 | 2.7132879841 |
| H15 | -4.4016900439 | -7.0063189741 | 1.2193067173 |
| H16 | -2.9048857412 | -5.2283405228 | 0.4138664657 |
| O17 | 0.6683183171 | 2.0869322650 | 4.3344392260 |
| N18 | 0.6605244596 | 0.8527737950 | 1.2166271377 |
| H19 | -2.1897150467 | -0.1887190997 | -0.6828610857 |
| H20 | -0.1254350649 | 0.5591591704 | 0.5996625664 |
| H21 | 1.4250137136 | 0.1846346063 | 1.1475322666 |
| H22 | 0.9931808045 | 1.7468618215 | 0.8556391682 |

**19**

Energy = -956.244177 h

Zero Point Energy (ZPE): 62.935 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.5650531945 | 0.2062473410 | -0.2391204510 |
| O2 | 2.4256633566 | -0.2642123254 | -0.0352973655 |
| O3 | 0.2419186443 | 1.6841876293 | -1.0281454472 |
| O4 | -0.0778205089 | 0.1087997506 | 1.5712069522 |

| | | | |
|---|---|---|---|
| N5 | -0.2196338063 | -1.0485624668 | -1.2017350399 |
| Mo6 | 0.4168044641 | -1.1120024504 | 2.9686760753 |
| O7 | 2.2860622675 | -1.5003437149 | 2.6528707166 |
| Mo8 | 3.1451052895 | -1.7201055052 | 0.9682585520 |
| O9 | 0.0307205281 | -0.6750474797 | 4.5696095646 |
| N10 | -0.4348472092 | -2.7356023860 | 2.5892845512 |
| C11 | -1.4522528365 | -3.8863285407 | 4.4835232668 |
| C12 | -1.0983037773 | -3.7278403274 | 3.0878985765 |
| H13 | -1.4111172414 | -4.5211729554 | 2.3980810812 |
| C14 | -2.1140039373 | -4.9718922855 | 4.9256170517 |
| H15 | -2.4103942397 | -5.7701604248 | 4.2498528866 |
| H16 | -2.3730285153 | -5.0921361952 | 5.9721339826 |
| H17 | -1.1553311332 | -3.0917143094 | 5.1640479891 |
| O18 | 4.8465032581 | -1.6882108049 | 1.0911329768 |
| O19 | 2.6510624347 | -3.1936638409 | 0.2492205708 |
| H22 | -0.2409540049 | -2.0659989789 | -1.0809185593 |

**TS12**

Energy = -956.205042 h

Zero Point Energy (ZPE): 60.168 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.6401054769 | 0.7098885338 | 0.0265191817 |
| O2 | 1.8555232138 | -0.6801439231 | -0.4444660581 |
| O3 | 1.4233994990 | 2.1964156839 | 0.3091512825 |
| O4 | -0.3095814127 | 0.1118497469 | 1.6198588560 |
| N5 | -0.5126454822 | 0.9007548224 | -1.2942986674 |
| Mo6 | 0.2845866840 | -1.3650732589 | 2.6671450365 |
| O7 | 2.1363853336 | -1.2988069406 | 2.2533847866 |
| Mo8 | 2.8544064438 | -1.9953604966 | 0.5778185309 |
| O9 | 0.0618724096 | -1.4895422070 | 4.3494130690 |
| N10 | -0.2382336453 | -2.9712538073 | 1.8313427849 |
| C11 | -1.2421846708 | -4.7443310016 | 0.5155802233 |
| C12 | -0.1492546715 | -3.9663232564 | 1.0752755467 |
| H13 | 1.2438370493 | -4.0090899968 | 0.5496308038 |
| C14 | -0.9818812483 | -5.8029080629 | -0.2684095922 |
| H15 | 0.0390534988 | -6.0893707026 | -0.5038272633 |
| H16 | -1.7806021019 | -6.4064426526 | -0.6878790624 |
| H17 | -2.2632243355 | -4.4531176911 | 0.7579499389 |
| O18 | 4.5425531020 | -1.7907229963 | 0.6262713941 |
| O19 | 2.2538238636 | -3.6751716848 | 0.1546555618 |
| H20 | -0.8154782675 | 1.6875582102 | -1.8705879846 |

Energy = -956.216380 h
Zero Point Energy (ZPE): 61.843 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5537014249 | 0.2976691596 | 0.7249862478 |
| O2 | -1.8998773036 | 1.8065567642 | 1.8111923013 |
| O3 | -3.4403413308 | 0.6510824176 | -0.6963004583 |
| O4 | -3.5246605812 | -0.5844488237 | 2.0747038255 |
| N5 | -1.0846363691 | -0.5909307009 | 0.2484730777 |
| Mo6 | -3.1525422115 | -1.0818885037 | 3.9283480616 |
| O7 | -2.0755485143 | 0.3970054640 | 4.4636520257 |
| Mo8 | -1.0395930339 | 1.6984423197 | 3.4809158131 |
| O9 | -4.4534607947 | -1.6488580604 | 4.8564035300 |
| N10 | -2.1281254427 | -2.7860678281 | 3.4074468476 |
| H11 | -0.3448837148 | -0.9695318513 | 0.8460713567 |
| C12 | -0.9254727481 | -4.9920816156 | 2.8073963673 |
| C13 | -1.5925995409 | -3.7884242365 | 3.1319844853 |
| C15 | -1.1305323077 | -6.1407400605 | 3.4775313136 |
| H16 | -1.8097709631 | -6.2025061581 | 4.3209809018 |
| H17 | -0.6194366306 | -7.0470568027 | 3.1739298506 |
| H18 | -0.2483171503 | -4.9340978507 | 1.9588836981 |
| O19 | 0.5660162525 | 0.6486912015 | 3.2918946721 |
| O20 | -0.7583538029 | 3.0908969581 | 4.4162929063 |
| H22 | 0.7721124538 | 0.0223606683 | 4.0025630134 |

**21** (one Mo-Mo bond)
Energy = -785.368101 h
Zero Point Energy (ZPE): 30.165 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5340921378 | 0.0020301709 | 0.8246458825 |
| O2 | -1.6609059582 | 1.5545251747 | 1.6422737873 |
| O3 | -3.9942173934 | 0.4561948323 | 0.0766014699 |
| O4 | -2.8139246612 | -1.3964273551 | 2.1231603233 |
| N5 | -1.4364140406 | -0.6313350002 | -0.3942981097 |
| Mo6 | -2.8371199087 | -0.6879369607 | 3.9123446166 |
| O7 | -1.2073487753 | 0.0435816945 | 4.6497127059 |
| Mo8 | -1.1725217196 | 1.5375135974 | 3.4685721497 |
| O9 | -4.2692101224 | -0.2308487952 | 4.6902723218 |
| H10 | -1.4166595149 | -0.8032831066 | -1.3994511815 |
| H11 | 1.2124593777 | 2.3843939548 | 3.5744767276 |
| O12 | 0.7321846966 | 1.5657934992 | 3.3788897114 |
| O13 | -1.9290116328 | 2.8330636332 | 4.2496364349 |

**21** (no Mo-Mo bonds)
Energy = -785.348248 h

Zero Point Energy (ZPE): 29.480 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.3481897703 | 0.0452526364 | 0.7151978502 |
| O2 | -1.3656730379 | 1.3245372556 | 1.7682514926 |
| O3 | -3.4939366525 | 0.8053456675 | -0.2900601593 |
| O4 | -3.1704926166 | -1.1733230049 | 1.9529924541 |
| N5 | -1.1982602393 | -0.8442863805 | -0.2803900054 |
| Mo6 | -3.3862156767 | -0.8882716821 | 3.8385096159 |
| O7 | -2.2784251081 | 0.5699917929 | 4.3720197178 |
| Mo8 | -0.9790311113 | 1.7332227590 | 3.5972240939 |
| O9 | -4.8099176875 | -1.2331114005 | 4.6815851253 |
| H11 | -1.0661487895 | -0.9933059925 | -1.2819422924 |
| O19 | 0.7375436937 | 1.0939051840 | 4.1150935623 |
| O20 | -1.3347042806 | 3.2847321632 | 4.1821174511 |
| H22 | 0.9092578427 | 0.1884249115 | 4.4138170838 |

## Ammoxidation of allyl on $Mo3O_6(NH)_3$ - Figure 9

**22**
Energy = -820.251137 hartrees
Zero Point Energy (ZPE): 39.106 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7192647691 | 0.5433874223 | 0.8126768293 |
| O2 | -0.9360064674 | 0.6572658560 | 1.5127053303 |
| N3 | -3.4720268674 | 2.1317500164 | 0.8884964942 |
| O4 | -3.6107884680 | -0.6358915103 | 2.0362321247 |
| O5 | -2.7573948859 | -0.0267712793 | -0.7906240691 |
| Mo6 | -3.3976263211 | -0.8543821682 | 3.9308505192 |
| O7 | -1.5231135745 | -0.5542920135 | 4.2114971377 |
| Mo8 | -0.3082769131 | 0.6385807756 | 3.3261216636 |
| O9 | -3.9044501508 | -2.3858989087 | 4.4740149750 |
| N10 | -0.4765462064 | 2.2493434791 | 4.0132085014 |
| O11 | 1.3126065068 | 0.1344124274 | 3.4523937029 |
| N12 | -4.3137302745 | 0.3956818161 | 4.7633003842 |
| H13 | -5.0500625669 | 0.4514996029 | 5.4675962102 |
| H14 | 0.1196972930 | 2.9484434597 | 4.4571663299 |
| H15 | -3.9155813436 | 2.7901198254 | 0.2473968866 |

**23**
Energy = -937.574560
Zero Point Energy (ZPE): 85.122 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5839628120 | 0.6311132574 | 0.7454645931 |

| | | | |
|---|---|---|---|
| O2 | -2.0302995417 | 2.0312161901 | 1.9338491609 |
| O3 | -3.6997252116 | 1.1734548864 | -0.4243855981 |
| O4 | -3.2980255217 | -0.7165751261 | 1.8800600840 |
| N5 | -1.1450427113 | -0.0423819634 | -0.0389257350 |
| Mo6 | -2.7621445877 | -1.4907674229 | 3.5750507735 |
| O7 | -1.6008416628 | -0.0317905494 | 4.0972349873 |
| Mo8 | -1.2852845339 | 1.8017275063 | 3.6901834952 |
| O9 | -4.1119122864 | -1.6479680218 | 4.5957087199 |
| N10 | -1.6821871714 | -3.0687416922 | 3.2965278679 |
| H11 | -1.9170753200 | -3.9310363709 | 3.7877556015 |
| C12 | 0.7175380338 | -3.6320258539 | 3.2866655283 |
| C13 | -0.4737401933 | -3.2163162535 | 2.4630845135 |
| H14 | -0.2866898053 | -2.2572419697 | 1.9644618497 |
| H15 | -0.6707709904 | -3.9556631569 | 1.6755030286 |
| C16 | 1.3729933990 | -4.7812603475 | 3.1190261703 |
| H17 | 1.0829544615 | -5.5000618490 | 2.3557179746 |
| H18 | 2.2324751438 | -5.0407149023 | 3.7299462010 |
| H19 | 1.0284055849 | -2.9271130840 | 4.0565603425 |
| N20 | 0.4607093881 | 2.0701750806 | 3.6548411887 |
| O21 | -2.0066899646 | 2.8676239109 | 4.8095596323 |
| H22 | -0.8457355115 | -0.1233996377 | -1.0114766154 |
| H23 | 1.0826124549 | 2.7370361383 | 4.1143920859 |

**23** (another conformer)
Energy = -937.558953
Zero Point Energy (ZPE): 84.637 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9168803622 |
| O3 | 1.5646858508 | 0.0000000000 | -0.6713115398 |
| O4 | -1.0030546293 | 1.5845806520 | -0.4284906549 |
| N5 | -0.9064665615 | -1.4120106710 | -0.5586155138 |
| Mo6 | -2.4921470796 | 2.3303136959 | 0.5399253650 |
| O7 | -2.1576048467 | 1.9956234117 | 2.4036888443 |
| Mo8 | -1.4401121493 | 0.3687910924 | 3.1384630538 |
| O9 | -3.0666345912 | 3.8826635663 | 0.1366755890 |
| N10 | -3.9276515521 | 1.0353044801 | 0.2640758072 |
| H11 | -4.6603215663 | 1.0135253415 | 0.9728738135 |
| C12 | -5.0726529569 | 1.6474530313 | -1.8691870473 |
| C13 | -4.3900238206 | 0.5736761280 | -1.0596392238 |
| H14 | -5.0723878660 | -0.2713832816 | -0.8903489310 |
| H15 | -3.5265614986 | 0.1815226167 | -1.6078943494 |
| C16 | -4.6458597854 | 2.0615773856 | -3.0627468117 |
| H17 | -3.7662867890 | 1.6298872787 | -3.5355139633 |
| H18 | -5.1611133961 | 2.8426108818 | -3.6133776857 |
| H19 | -5.9546531416 | 2.1011911789 | -1.4174691862 |

| | | | |
|---|---|---|---|
| N20 | -2.6653736200 | -0.9053427902 | 2.9546304931 |
| O21 | -1.0535122960 | 0.4230726239 | 4.7988815292 |
| H22 | -0.7030920180 | -2.2074243063 | -1.1659394119 |
| H23 | -3.0409569906 | -1.1349756814 | 2.0242259079 |

**TS13**

E= -937.533347

Zero Point Energy (ZPE): 82.010 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1924669843 | 0.3458705640 | 0.0760771160 |
| O2 | -0.1084668473 | -0.2728415879 | 1.8485207934 |
| O3 | 1.8194269009 | 0.5883397823 | -0.3700269664 |
| O4 | -0.7970991166 | 1.9323794774 | 0.1034739292 |
| N5 | -0.6847997851 | -0.8165869300 | -1.0859182558 |
| Mo6 | -2.7656253539 | 2.0149356525 | -0.0312919418 |
| H7 | -1.8717012432 | -0.7037905077 | -1.4216618060 |
| C8 | -3.2852047148 | -0.5202281557 | -1.6479998086 |
| O9 | -3.2292789884 | 3.6342930132 | -0.2450827727 |
| N10 | -3.5495553400 | 0.8281148893 | -1.3854670730 |
| C11 | -3.6115561582 | -1.0731591802 | -2.9675297304 |
| Mo12 | -1.6815030088 | 0.2697289828 | 2.8649661216 |
| H13 | -3.5055126846 | -1.1619291308 | -0.7890167900 |
| O14 | -2.9369307148 | 0.9212732775 | 1.6012648528 |
| C15 | -3.6997397775 | -0.3919847109 | -4.1222334322 |
| H16 | -3.5233485928 | 0.6794157769 | -4.1890292631 |
| H17 | -3.9419845375 | -0.8938613939 | -5.0523558557 |
| H18 | -3.7523831720 | -2.1529287032 | -2.9834080419 |
| O19 | -1.2782085857 | 1.4394553414 | 4.0391459747 |
| N20 | -2.3647176434 | -1.1496863251 | 3.6607398829 |
| H21 | -0.2142112605 | -1.3260873356 | -1.8351885391 |
| H22 | -4.0225620962 | 1.2996776697 | -2.1597528279 |
| H23 | -2.5163546927 | -1.4136767280 | 4.6351448972 |

**24**

Energy = -937.584638 h

Zero Point Energy (ZPE): 85.881 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1477063271 | -0.0010740498 | -0.0165330787 |
| O2 | 2.0770347129 | -0.1613893412 | -0.2312070976 |
| O3 | -0.7199875595 | 1.0588192303 | -1.0382714115 |
| O4 | -0.0652597899 | 0.0498523980 | 1.8425280861 |
| N5 | -0.2724365465 | -1.9248381630 | -0.4354105662 |
| Mo6 | 0.8037610605 | -1.1606061146 | 3.1621884679 |
| O7 | 2.5758909497 | -1.3711090272 | 2.4368247035 |
| Mo8 | 3.2196947766 | -1.4222120572 | 0.6186342271 |
| O9 | 0.4028571360 | -1.0862025039 | 4.8118622712 |

| | | | |
|---|---|---|---|
| N10 | -0.3509856031 | -2.7176580418 | 2.4579348923 |
| C11 | -1.4556363292 | -3.7822533276 | 4.3461681466 |
| C12 | -1.1579306524 | -3.6155584985 | 2.9423261319 |
| H13 | -1.6481846957 | -4.2894274468 | 2.2370146390 |
| C14 | -2.3084260338 | -4.7259192100 | 4.7819213337 |
| H15 | -2.8128781207 | -5.4014171307 | 4.0953242982 |
| H16 | -2.5269254353 | -4.8482605500 | 5.8372502489 |
| H17 | -0.9628669667 | -3.1087895448 | 5.0425235105 |
| O18 | 4.8776587373 | -1.0419947749 | 0.4824797166 |
| N19 | 2.8782389976 | -3.0366421069 | -0.0508230854 |
| H20 | -0.3027140997 | -2.7024271271 | 1.4176331219 |
| H21 | 0.4209772268 | -2.4343793649 | -0.9830078410 |
| H22 | -1.2063161146 | -2.1341689922 | -0.7808446245 |
| H23 | 3.4806198753 | -3.7477482978 | -0.4685741342 |

**TS14**

Energy = -937.573570 h

Zero Point Energy (ZPE): 83.352 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9425787239 |
| O3 | 1.4427314562 | 0.0000000000 | -0.9126922808 |
| O4 | -1.4322156695 | 1.1547312764 | -0.3675039078 |
| N5 | -1.1337851041 | -1.7676503359 | -0.2922535381 |
| Mo6 | -3.2243348395 | 1.0468431005 | 0.4415146095 |
| O7 | -2.8897305499 | 0.6036177247 | 2.2973282948 |
| Mo8 | -1.4773436823 | -0.4438245570 | 3.0700680525 |
| O9 | -4.5187657711 | 1.9963903904 | -0.1125503457 |
| N10 | -3.4914488966 | -0.6993796709 | -0.5180471140 |
| H11 | -2.3623159021 | -1.3609790620 | -0.4111821036 |
| C12 | -4.4422562819 | -2.4231148253 | -1.9352082511 |
| C13 | -4.4221262285 | -1.1089644185 | -1.3127737483 |
| H14 | -1.0953334086 | -2.4014332822 | 0.5124232709 |
| H15 | -5.2548635036 | -0.4385824169 | -1.5532455956 |
| C16 | -5.4117425422 | -2.8019099651 | -2.7838003998 |
| H17 | -6.2318970886 | -2.1354096648 | -3.0384203863 |
| H18 | -5.4157925407 | -3.7832956674 | -3.2455597786 |
| H19 | -3.6307016597 | -3.1043022588 | -1.6859684088 |
| N20 | -1.8404344018 | -2.1697645563 | 2.7869476955 |
| O21 | -1.2286337818 | -0.1182191758 | 4.7257942175 |
| H22 | -0.8570993913 | -2.2804126334 | -1.1296856181 |
| H23 | -1.9375224027 | -2.9498039212 | 3.4390939067 |

**25**

Energy = -937.579291 h

Zero Point Energy (ZPE): 86.213 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.9631624162 | 0.5612438080 | 0.7681217868 |
| O2 | -2.3142238993 | 1.9978657314 | 1.9705069833 |
| O3 | -3.6899517499 | 0.7229591365 | -0.7608687666 |
| O4 | -3.5359924022 | -0.7823976705 | 2.0828103655 |
| N5 | -0.9974405263 | -0.4599805390 | 0.5965480194 |
| Mo6 | -2.7549239342 | -1.2787260314 | 3.7228597980 |
| O7 | -1.9191421067 | 0.3364135034 | 4.3795483152 |
| Mo8 | -1.1231594989 | 1.7932676861 | 3.4204184635 |
| O9 | -3.6713233600 | -2.2790523553 | 4.7597145477 |
| N10 | -1.3489031829 | -2.4278586256 | 3.0708548012 |
| H11 | -0.9988636355 | -1.3374428279 | 1.1322665381 |
| C12 | 0.1149377593 | -4.3401488340 | 2.8394166544 |
| C13 | -1.0783457353 | -3.6657174891 | 3.3215170964 |
| H14 | -0.2621154922 | 0.1238179551 | 1.0255465133 |
| H15 | -1.7640757166 | -4.2691122641 | 3.9354214175 |
| C16 | 0.3665815299 | -5.6321784156 | 3.1137960011 |
| H17 | -0.3222430311 | -6.2264718813 | 3.7091072947 |
| H18 | 1.2615487515 | -6.1302145292 | 2.7564592592 |
| H19 | 0.8087353193 | -3.7469281452 | 2.2475537470 |
| N20 | 0.4232993069 | 1.2134844829 | 2.7167974736 |
| O21 | -0.8991593377 | 3.1893741074 | 4.3771774923 |
| H22 | -0.7435563823 | -0.6608796459 | -0.3696832787 |
| H23 | 1.3711280775 | 1.5623673940 | 2.8692580348 |

**TS15**

Energy = -937.528788 h

Zero Point Energy (ZPE): 83.029 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.0509151770 | -0.1067428217 | -0.0085828074 |
| C2 | 0.0487832179 | -0.0346233885 | 1.3290945470 |
| C3 | 1.2594255070 | 0.0196623155 | 2.1429035854 |
| N4 | 1.3703186169 | 0.0496429474 | 3.3794883474 |
| Mo5 | 3.0183089998 | -0.2235023574 | 4.5173831310 |
| O6 | 2.3484924523 | -0.6753673913 | 6.0195278036 |
| O7 | 4.0092821916 | 1.3831299338 | 4.4546997709 |
| Mo8 | 5.5256188404 | 2.1206293473 | 3.4566384868 |
| N9 | 4.1342121831 | 2.8104058268 | 1.8830724615 |
| O10 | 6.1664975970 | 0.4985063253 | 2.5405238688 |
| Mo11 | 5.0601449066 | -0.8938815900 | 1.8798608463 |

| | | | |
|---|---|---|---|
| O12 | 5.6762414034 | -2.2481010278 | 1.0413140154 |
| O13 | 6.4345365965 | 3.4321550411 | 4.0492837358 |
| O14 | 4.0965139280 | -1.3944072657 | 3.4881920469 |
| N15 | 3.6347784645 | 0.0142795583 | 0.9294257985 |
| H16 | 3.2680974729 | 3.1945724235 | 2.2603809948 |
| H17 | 3.8964238430 | 1.9480018463 | 1.3507472817 |
| H18 | 2.5403363814 | 0.0223385673 | 1.3777885067 |
| H19 | 0.9741366930 | -0.1242202053 | -0.5799590282 |
| H20 | -0.8755410793 | -0.1617706321 | -0.5700435739 |
| H21 | -0.8875103463 | -0.0286617801 | 1.8874797422 |
| H22 | 4.5329667926 | 3.4912595754 | 1.2388766192 |
| H23 | 3.5260891747 | -0.1851680081 | -0.0663526395 |

**26**

Energy = -937.572804 h

Zero Point Energy (ZPE): 86.060 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7916422417 | 0.4264555925 | 0.7344081780 |
| O2 | -2.1084602756 | 1.8749207798 | 1.9114435917 |
| O3 | -3.7232312960 | 0.9003147875 | -0.6122762262 |
| O4 | -3.2751988109 | -0.8669111961 | 1.9970092397 |
| N5 | -0.6647179387 | 0.3601832129 | 0.1125680118 |
| Mo6 | -2.9510447656 | -1.2635072074 | 3.9107543906 |
| O7 | -1.9724546660 | 0.2763630606 | 4.4079052799 |
| Mo8 | -1.0723149391 | 1.7312951520 | 3.4513434180 |
| O9 | -4.3204646639 | -1.8374457949 | 4.7430416210 |
| N10 | -1.8902846682 | -2.9664155175 | 3.4979161473 |
| H11 | -0.1209609442 | 0.2581476390 | 1.0002750465 |
| C12 | -0.8262601654 | -5.3066953862 | 3.2459206501 |
| C13 | -1.4139489384 | -4.0303735617 | 3.3684723857 |
| H14 | -0.3983784823 | 1.2607154279 | -0.2860791405 |
| H15 | 0.7437291607 | -0.1841581784 | 3.4485442055 |
| C16 | -1.3997655583 | -6.4356934748 | 3.7077746106 |
| H17 | -2.3590491427 | -6.4281096907 | 4.2134814406 |
| H18 | -0.9054340722 | -7.3909659670 | 3.5765787497 |
| H19 | 0.1347325445 | -5.3260009910 | 2.7374532724 |
| N20 | 0.5084211115 | 0.5853920868 | 2.8226286126 |
| O21 | -0.5979719815 | 3.1284822590 | 4.3208409543 |
| H22 | -0.3961753816 | -0.3682628775 | -0.5441427927 |
| H23 | 1.3675937097 | 1.1012633780 | 2.6389359996 |

**TS16**

Energy = -937.5656267 h
Zero Point Energy (ZPE): 81.962 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| C2 | 0.0000000000 | 0.0000000000 | 1.3438458903 |
| C3 | 1.2345003263 | 0.0000000000 | 2.1076886993 |
| N4 | 1.2826254269 | 0.0049089868 | 3.4002436647 |
| Mo5 | 2.8633725788 | 0.1423576177 | 4.6766912507 |
| O6 | 4.2402573659 | 0.6963468796 | 3.8342713998 |
| O7 | 3.0668005920 | -1.6626315615 | 5.3220789506 |
| Mo8 | 1.9558801745 | -2.5833358471 | 6.5995146925 |
| N9 | 0.6808611135 | -3.7270052477 | 5.6612340524 |
| O10 | 0.9634654085 | -1.1377754611 | 7.2823889002 |
| Mo11 | 0.2073988390 | 0.5534446428 | 6.7096859362 |
| O12 | -0.4385897416 | 1.5214672819 | 7.9615305602 |
| O13 | 2.8897327238 | -3.3506978401 | 7.7971979259 |
| O14 | 1.9657639346 | 1.1184816833 | 5.9889751490 |
| N15 | -0.6755214893 | 0.2752682705 | 5.0770103838 |
| H16 | 0.2301834404 | 0.0736951478 | 4.0900532399 |
| H17 | -0.1130593643 | -3.4052347235 | 5.1146062833 |
| H18 | 2.1669060778 | -0.0009337158 | 1.5337789223 |
| H19 | 0.9283665870 | 0.0034795098 | -0.5656538086 |
| H20 | -0.9220891935 | -0.0018529571 | -0.5711925819 |
| H21 | -0.9329917784 | -0.0030059206 | 1.9028411788 |
| H22 | 0.6728768843 | -4.7370824041 | 5.7637179480 |
| H23 | -1.5945591498 | 0.6505905194 | 4.8367057919 |

**28**

Energy = -937.591860 h
Zero Point Energy (ZPE): 83.997 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6505833413 | 0.7185713489 | 0.5902284740 |
| O2 | -1.6010257998 | 1.5016288795 | 1.9775598532 |
| O3 | -3.9860080064 | 1.7150468336 | 0.2433551487 |
| O4 | -3.1870007173 | -0.8227191200 | 1.6163145413 |
| N5 | -1.5246136770 | 0.1697362933 | -0.9058925052 |
| Mo6 | -3.0083239210 | -1.3858380503 | 3.4407981933 |
| O7 | -1.8829043973 | -0.0833856435 | 4.2904967144 |
| Mo8 | -0.9581328873 | 1.5044469402 | 3.7759259786 |
| O9 | -4.4339218444 | -1.5603420397 | 4.3660674104 |
| N10 | -2.0230316485 | -2.9941229540 | 3.4981077417 |
| H11 | 1.4462342034 | 0.3558476379 | 3.4380433526 |
| C12 | -1.2108960536 | -5.2631724045 | 3.5618572615 |

| | | | |
|---|---|---|---|
| C13 | -1.9366452363 | -4.1296981840 | 4.1053025276 |
| H14 | -0.6514919695 | -0.3469948038 | -0.8443696975 |
| H15 | -2.4234755812 | -4.2755263496 | 5.0804359918 |
| C16 | -1.1355089383 | -6.4472073840 | 4.1970403998 |
| H17 | -1.6184853745 | -6.6059653633 | 5.1580436847 |
| H18 | -0.5940761428 | -7.2877616454 | 3.7758136802 |
| H19 | -0.7284145796 | -5.1110595686 | 2.5989154986 |
| N20 | 0.9680032214 | 1.1671058848 | 3.8198603018 |
| O21 | -1.5376292835 | 2.8366981620 | 4.6607730611 |
| H22 | -1.7332155331 | 0.4117765952 | -1.8701585851 |
| H23 | 1.6195445885 | 1.7703643100 | 4.3130014581 |

**TS17**

Energy = -937.533221 h

Zero Point Energy (ZPE): 82.551 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | -0.0111771851 | 0.2902832519 | 0.0391128122 |
| C2 | 0.1622077506 | 0.3493415573 | 1.3679379295 |
| C3 | 1.3385517327 | -0.2328168533 | 2.0152133662 |
| N4 | 1.5549290904 | -0.1672816112 | 3.2560545484 |
| Mo5 | 2.7948436209 | -0.1948197998 | 4.7067116018 |
| O6 | 2.0681868336 | -0.9022300609 | 6.0786999891 |
| O7 | 3.6735002632 | 1.4794504618 | 4.7429169993 |
| Mo8 | 5.0811081745 | 2.1218713448 | 3.5329115467 |
| N9 | 3.8418949197 | 2.6025604125 | 2.0380097897 |
| O10 | 5.9702616137 | 0.5526583797 | 2.9596254392 |
| Mo11 | 5.2060686657 | -1.1637049086 | 2.4303648681 |
| O12 | 6.1921623957 | -2.5043510605 | 2.0785242356 |
| O13 | 5.9821449814 | 3.4286540704 | 4.1566589638 |
| O14 | 4.1314075736 | -1.3528625885 | 4.0419714655 |
| N15 | 3.7748055857 | -0.5163630056 | 0.9651920753 |
| H16 | 2.8634171602 | 2.7782549292 | 2.2583871957 |
| H17 | 3.8957898646 | 0.4943692973 | 0.8172389317 |
| H18 | 2.5798172890 | -0.5724506553 | 1.3207652895 |
| H19 | 0.7169999708 | -0.1947673387 | -0.6044317916 |
| H20 | -0.8860236311 | 0.7183675606 | -0.4397245438 |
| H21 | -0.5797231433 | 0.8295809908 | 2.0057112197 |
| H22 | 4.1558019935 | 3.2859930007 | 1.3526704885 |
| H23 | 3.8514203172 | -0.9873489828 | 0.0629113435 |

**Acrylonitrile ($NCCHCH_2$)**

Energy = -170.831737 h
Zero Point Energy (ZPE): 31.919 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| N10 | -1.8901790706 | -2.9628423705 | 3.4886842466 |
| C12 | -0.8242528072 | -5.3153734415 | 3.2448360668 |
| C13 | -1.4231056686 | -4.0233819979 | 3.3856505277 |
| C16 | -1.3936193272 | -6.4369089061 | 3.7027574526 |
| H17 | -2.3519768630 | -6.4256238058 | 4.2110799068 |
| H18 | -0.9042300694 | -7.3966281959 | 3.5753914118 |
| H19 | 0.1369253160 | -5.3379205277 | 2.7374303011 |

**27** (one Mo-Mo bond)
Energy = -766.713701 hartrees
Zero Point Energy (ZPE): 53.937 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.4565624469 | 0.4391523116 | 0.7065360270 |
| O2 | -1.7909607864 | 1.8104641033 | 1.8286793708 |
| O3 | -3.3667758097 | 0.7625964523 | -0.6990790804 |
| O4 | -3.4018675317 | -0.6839886220 | 1.9063494677 |
| N5 | -0.8158597653 | -0.6904552758 | 0.4001664075 |
| Mo6 | -3.0908566369 | -0.8439175135 | 3.7778804625 |
| O7 | -1.2959979776 | -0.5214918405 | 4.3267739137 |
| Mo8 | -1.3625670091 | 1.3348949733 | 3.7081274325 |
| O9 | -4.4333766213 | -0.7727746919 | 4.8182117601 |
| H11 | 0.3868555729 | 0.2114548204 | 1.9995933432 |
| H14 | -0.2681467167 | -0.4888068465 | -0.4344780261 |
| H15 | 1.1938357082 | 0.2056523896 | 3.4573146798 |
| N20 | 0.6393155046 | 0.7815230032 | 2.8266241706 |
| O21 | -1.5200604908 | 2.5823277981 | 4.8473150671 |
| H22 | -0.8776328019 | -1.7015350128 | 0.5017293899 |
| H23 | 1.2011932345 | 1.5700920979 | 2.5117224035 |

**27** (two Mo-Mo bonds)
Energy = -766.745037 hartrees
Zero Point Energy (ZPE): 54.084 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7801800120 | 0.0928056668 | 1.1704420118 |
| O2 | -1.2920384323 | 1.3553243076 | 1.5574569247 |
| O3 | -4.2775728721 | 0.6390901836 | 0.5781336840 |
| O4 | -2.6394317106 | -1.6270402554 | 2.0948215747 |
| N5 | -1.3916318820 | -0.8875255389 | -0.3368967326 |
| Mo6 | -2.6899065600 | -0.6324702415 | 3.7501706722 |
| O7 | -0.9716927324 | -0.1594768039 | 4.4614673169 |

| | | | |
|---|---|---|---|
| Mo8 | -1.0772669579 | 1.5098255289 | 3.4431838351 |
| O9 | -4.1491111586 | -0.2699525985 | 4.5515909426 |
| H10 | -1.7467546406 | -0.8992847528 | -1.2913619870 |
| H11 | 1.2663669739 | 2.5231116264 | 3.9817377245 |
| N12 | 0.8376815309 | 1.6129012162 | 3.8377375064 |
| O13 | -1.8699964248 | 2.8217684455 | 4.1925633283 |
| H14 | 1.3330861864 | 0.8815663197 | 4.3384749113 |
| H15 | -0.4962061938 | -0.3996864805 | -0.3322745073 |
| H16 | -1.2438439821 | -1.8496486675 | -0.0326191453 |

**27** (no Mo-Mo bonds)
Energy = -766.705115 hartrees
Zero Point Energy (ZPE): 53.364 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.8387197434 | 0.8928868501 | 0.7975468562 |
| O2 | -1.8720236777 | 2.0232633303 | 2.1489599850 |
| O3 | -3.5038929142 | 1.5252281557 | -0.6324440977 |
| O4 | -3.3948912476 | -0.7275127316 | 1.7263083324 |
| N5 | -0.8785525983 | 0.0392790698 | 0.2526070829 |
| Mo6 | -3.1739122304 | -1.2325423445 | 3.5397191222 |
| O7 | -2.0010586563 | -0.0278981339 | 4.4415288035 |
| Mo8 | -0.9854609394 | 1.4430507687 | 3.6883723195 |
| O9 | -3.8794962019 | -2.6146277709 | 4.2350870022 |
| H11 | -0.3142495848 | 0.0052934197 | 1.1340592656 |
| H14 | -0.3779834771 | 0.6225021995 | -0.4164648036 |
| N12 | 0.4570813467 | 0.2634791459 | 2.8852428285 |
| O20 | -0.2600613203 | 2.5373894003 | 4.7806596623 |
| H21 | -0.9417477113 | -0.9018678670 | -0.1332804464 |
| H22 | 0.6538264521 | -0.5882737276 | 3.4095379122 |
| H16 | 1.3434121670 | 0.7288930372 | 2.6944717734 |

**29**
Energy = -936.350662 hartrees
Zero Point Energy (ZPE): 69.548 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.9014593677 | 0.5077670751 | 0.7627688172 |
| O2 | -2.2604136944 | 1.9280719493 | 1.8932054377 |
| O3 | -4.0153745563 | 0.9446560056 | -0.4556474423 |
| O4 | -3.5521505156 | -0.7437450277 | 2.0659408985 |
| N5 | -1.5013978801 | -0.1957560318 | -0.0654366940 |
| Mo6 | -2.7505988117 | -1.2736202770 | 3.7287136462 |
| O7 | -1.8853635764 | 0.3137376184 | 4.3851079929 |
| Mo8 | -1.1060610935 | 1.7793558201 | 3.4168504724 |

| | | | |
|---|---|---|---|
| O9 | -3.7758887862 | -2.1083600243 | 4.8018842795 |
| N10 | -1.4055758108 | -2.4940670538 | 3.2396423254 |
| H11 | -0.6496857807 | -0.5490155845 | 0.3855157787 |
| C12 | 0.0895889620 | -4.3579653408 | 2.9138935213 |
| C13 | -1.0968453999 | -3.7319625876 | 3.4574892767 |
| H15 | -1.7536769604 | -4.3575595312 | 4.0793884187 |
| C16 | 0.3815886852 | -5.6523717379 | 3.1453894378 |
| H17 | -0.2655072013 | -6.2786361107 | 3.7542356516 |
| H18 | 1.2697148049 | -6.1191201707 | 2.7330980863 |
| H19 | 0.7370768384 | -3.7334173054 | 2.3035930705 |
| N20 | 0.4953245707 | 1.2984633414 | 2.8425130732 |
| O21 | -1.0001747292 | 3.2074388876 | 4.3384918236 |
| H23 | 1.4417337200 | 1.6690539627 | 2.9404321321 |

**TS18**

Energy = -936.317069 hartrees

Zero Point Energy (ZPE): 67.075 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.0286602156 | 0.0173005442 | 0.1720451641 |
| C2 | 1.3362359305 | 0.2755600063 | 0.3266848658 |
| C3 | 1.9693717656 | 1.3728716189 | -0.3952643816 |
| N4 | 3.1777362684 | 1.7051197970 | -0.3297603829 |
| Mo5 | 4.5682092915 | 3.0052324074 | -0.4494902230 |
| O6 | 5.9010200352 | 2.5425138340 | -1.3974595984 |
| O7 | 4.6029676915 | 3.9260322155 | 1.2898651666 |
| Mo8 | 3.3767500750 | 5.0765437948 | 2.1551312683 |
| N9 | 2.5410117349 | 4.1599343195 | 3.4167282947 |
| O10 | 2.0520510860 | 5.6222036188 | 0.8319374010 |
| Mo11 | 1.9508876566 | 5.1156446139 | -0.9946496441 |
| O12 | 1.4478883637 | 6.3724388469 | -2.0278205267 |
| O13 | 4.1504053112 | 6.4197145330 | 2.8620239953 |
| O14 | 3.7095892641 | 4.6065565071 | -1.2761389977 |
| N15 | 0.8153818122 | 3.6358129479 | -1.1327958558 |
| H16 | 2.4150157021 | 4.2921561079 | 4.4218133034 |
| H17 | 1.2165122087 | 2.4883477311 | -0.9356065425 |
| H18 | -0.5901995746 | 0.6157358757 | -0.4901923505 |
| H19 | -0.4564380859 | -0.7974928670 | 0.7002446918 |
| H20 | 1.9555801418 | -0.3278178781 | 0.9889312698 |
| H21 | -0.0583505659 | 3.6449788437 | -1.6591305080 |

**30**
Energy = -936.343209 hartrees
Zero Point Energy (ZPE): 69.753 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6122954720 | 0.2533036224 | 0.7416185669 |
| O2 | -2.0426076931 | 1.8305381307 | 1.7724192782 |
| O3 | -3.5385192992 | 0.5010426187 | -0.6768638595 |
| O4 | -3.4798260099 | -0.6551227678 | 2.1411899294 |
| N5 | -1.0811795542 | -0.5389961227 | 0.2707035040 |
| Mo6 | -3.0420040404 | -1.1135174284 | 3.9945158137 |
| O7 | -1.9595937162 | 0.3793678160 | 4.4750171315 |
| Mo8 | -1.1074200735 | 1.7576244206 | 3.4093227352 |
| O9 | -4.3294099664 | -1.6664118459 | 4.9498396834 |
| N10 | -2.0694366694 | -2.8407120581 | 3.4538315411 |
| H11 | -0.3756890423 | -0.7727300625 | 0.9819053296 |
| C12 | -0.9593178746 | -5.0946334423 | 2.8557609745 |
| C13 | -1.5743344261 | -3.8628058092 | 3.1759242326 |
| H15 | 0.8636939499 | 0.0613465895 | 3.7867962034 |
| C16 | -1.2691258802 | -6.2464221909 | 3.4788085813 |
| H17 | -2.0020607227 | -6.2902489183 | 4.2772765204 |
| H18 | -0.7908910454 | -7.1726249509 | 3.1817423267 |
| H19 | -0.2300045853 | -5.0540854706 | 2.0506271247 |
| N20 | 0.5385268904 | 0.7166259828 | 3.0799712722 |
| O21 | -0.7682291518 | 3.1987076179 | 4.2576282068 |
| H23 | 1.3312340753 | 1.1615955254 | 2.6243290621 |

**31** (one Mo-Mo bond)
Energy = -765.498838 h
Zero Point Energy (ZPE): 37.861 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5516024935 | 0.0056156438 | 0.7707273501 |
| O2 | -1.6207175440 | 1.4946510350 | 1.6078017233 |
| O3 | -3.9646227188 | 0.5270628025 | -0.0237476671 |
| O4 | -2.9338196568 | -1.3167263701 | 2.1149096695 |
| N5 | -1.4660851479 | -0.7240847697 | -0.4077788930 |
| Mo6 | -2.8179727546 | -0.6722334586 | 3.9314707631 |
| O7 | -1.0859897348 | -0.0886310169 | 4.5220124285 |
| Mo8 | -1.1962720542 | 1.5276082848 | 3.4628304202 |
| O9 | -4.1492926956 | -0.2635776334 | 4.8978507648 |
| H10 | -1.4607763899 | -0.9056466125 | -1.4116483470 |
| H11 | 1.2030948604 | 2.5227661985 | 3.7347420369 |
| N12 | 0.7384177264 | 1.6242130041 | 3.6386761959 |
| O13 | -1.9283747124 | 2.8335778956 | 4.2613109398 |
| H14 | 1.3237460052 | 0.8551006407 | 3.9501778621 |

**31** (no Mo-Mo bond)
Energy = -765.482045 h
Zero Point Energy (ZPE): 37.457 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| O2 | 0.0000000000 | 0.0000000000 | 1.9279347354 |
| O3 | 1.5933671546 | 0.0000000000 | -0.6004882609 |
| O4 | -1.0089584376 | 1.5038524347 | -0.6891753015 |
| N5 | -0.8006756518 | -1.4627023084 | -0.5593651477 |
| Mo6 | -1.2371178918 | 3.0720461754 | 0.3695647391 |
| O7 | -1.6649125040 | 2.7959892836 | 2.1792654767 |
| Mo8 | -0.7235755663 | 1.3563926819 | 3.0823399057 |
| O9 | -0.4517143793 | 4.5142499264 | -0.0371278525 |
| H10 | -0.5769022434 | -2.2821610830 | -1.1242646520 |
| H11 | -3.2507645466 | 1.1537617003 | 3.7846200985 |
| N12 | -2.3596193756 | 0.6758504241 | 3.8822681846 |
| O13 | 0.2990283658 | 1.9490560337 | 4.3052512949 |
| H14 | -2.3484339844 | 0.0554291131 | 4.6859123256 |

## Ammoxidation of allyl on $Mo_3O_3(NH)_6$ - Figure 10

**32**
Energy = -760.551960 hartree
Zero Point Energy (ZPE): 57.956 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6323346998 | 0.5443801279 | 0.8121092214 |
| O2 | -0.8464138114 | 0.6460200005 | 1.5327639986 |
| N3 | -3.3660748565 | 2.1305815638 | 0.7928358729 |
| O4 | -3.6328159147 | -0.6369753813 | 1.9625764280 |
| N5 | -2.5800482334 | -0.1140445708 | -0.8138914476 |
| Mo6 | -3.4492294404 | -0.8202656359 | 3.8736032679 |
| O7 | -1.5797782783 | -0.5769296042 | 4.2807681450 |
| Mo8 | -0.3529756139 | 0.6201775584 | 3.3971383307 |
| N9 | -3.9613488245 | -2.4243692734 | 4.3681636403 |
| N10 | -0.4822801348 | 2.2247814812 | 4.0764125819 |
| N11 | 1.2890440654 | 0.0234895545 | 3.5697473478 |
| N12 | -4.4070426744 | 0.3922817391 | 4.6904546753 |
| H13 | -5.1310673609 | 0.7330995892 | 5.3157990898 |

| | | | |
|---|---|---|---|
| H14 | -0.1570077824 | 3.0689650665 | 4.5376207476 |
| H15 | -3.8117192328 | 2.9399755195 | 0.3712987472 |
| H16 | 2.2237861203 | 0.2344754646 | 3.9122499208 |
| H17 | -4.6034508050 | -2.9599374674 | 4.9479925281 |
| H18 | -2.8069856667 | 0.0461090322 | -1.7927581933 |

**33**
Energy = -877.860008 hartree
Zero Point Energy (ZPE): 103.138 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5401412925 | 0.5181456435 | 0.7693920597 |
| O2 | -2.0506053582 | 1.9978417188 | 1.8980156875 |
| N3 | -3.6197750406 | 1.0442039083 | -0.5064738220 |
| O4 | -3.4035201043 | -0.7999811428 | 1.8613596880 |
| N5 | -1.0812592251 | -0.1927894691 | 0.0892013677 |
| Mo6 | -2.7332704577 | -1.3933917461 | 3.5896857197 |
| O7 | -1.4468431985 | -0.0416365272 | 4.1419732189 |
| Mo8 | -1.3244873328 | 1.8159086869 | 3.6810152167 |
| N9 | -4.1020272942 | -1.3828008874 | 4.6969147935 |
| N10 | -1.7011152481 | -3.0111034112 | 3.2710892110 |
| H11 | -1.9220350184 | -3.8587466055 | 3.7913676445 |
| C12 | 0.6718158907 | -3.6654278124 | 3.0844944150 |
| C13 | -0.5663054588 | -3.2143574551 | 2.3546457127 |
| H14 | -0.3815169046 | -2.2667240553 | 1.8334676227 |
| H15 | -0.8426124800 | -3.9517512929 | 1.5877274294 |
| C16 | 1.2914964006 | -4.8249672146 | 2.8605357576 |
| H17 | 0.9318364665 | -5.5291801539 | 2.1131374767 |
| H18 | 2.1870914015 | -5.1090401289 | 3.4052684528 |
| H19 | 1.0505873832 | -2.9754606823 | 3.8377790586 |
| N20 | 0.3640792208 | 2.3025395509 | 3.7404558906 |
| N21 | -2.2672770373 | 2.8055991537 | 4.7729127721 |
| H22 | -0.4944416837 | -0.4105692493 | -0.7110121034 |
| H23 | 1.0318230681 | 2.9757307885 | 4.1089692123 |
| H24 | -3.8031307593 | 1.1863869973 | -1.4959383514 |
| H25 | -4.5388579130 | -1.9348562322 | 5.4362634268 |
| H26 | -2.3835638503 | 3.5356872204 | 5.4690717768 |

**33** (another conformer)
Energy = -877.863801 h
Zero Point Energy (ZPE): 103.748 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1440582252 | 0.0997661739 | -0.1410138150 |
| O2 | 1.9330265528 | -0.5326202058 | -0.4466108051 |

| | | | |
|---|---|---|---|
| N3 | 0.1099267358 | 1.8491853521 | -0.1522535672 |
| O4 | -0.3961851104 | -0.5195077881 | 1.6174325604 |
| N5 | -0.9543146890 | -0.5185978895 | -1.3619962200 |
| Mo6 | 0.3711185097 | -2.1081115088 | 2.3841936830 |
| O7 | 2.3165746339 | -2.1194932944 | 2.1381488567 |
| Mo8 | 3.0703850125 | -1.8441202929 | 0.4024430698 |
| N9 | -0.2653027472 | -2.6018328951 | 3.9457003336 |
| N10 | 0.1096913540 | -3.5500292644 | 1.1114234257 |
| H11 | 0.9304456596 | -4.0528985848 | 0.7704130173 |
| C12 | -1.4692291837 | -5.4170743436 | 1.4936701276 |
| C13 | -1.1639954833 | -4.1609091188 | 0.7164220209 |
| H14 | -1.1202330954 | -4.3798877087 | -0.3608737341 |
| H15 | -1.9649982234 | -3.4280147038 | 0.8595506525 |
| C16 | -2.5336957446 | -5.5744903488 | 2.2814313160 |
| H17 | -3.2716188643 | -4.7850476701 | 2.4054511997 |
| H18 | -2.7131908025 | -6.4997004601 | 2.8215995606 |
| H19 | -0.7468223872 | -6.2275438843 | 1.3892232274 |
| N20 | 3.0476018388 | -3.3682944264 | -0.4979493515 |
| N21 | 4.7103070877 | -1.2711702213 | 0.5631470821 |
| H22 | -1.6042903900 | -0.3316186155 | -2.1211138930 |
| H23 | 3.6531850027 | -4.0134283017 | -1.0014542553 |
| H24 | -0.2101914772 | 2.7260614901 | -0.5542369561 |
| H25 | -0.4207922004 | -3.3947647155 | 4.5661317917 |
| H26 | 5.7066887156 | -1.2075747582 | 0.3811491671 |

**TS19**

Energy = -877.830237 h

Zero Point Energy (ZPE): 100.837 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | 0.1835359486 | 0.3990178457 | 0.1227245050 |
| O2 | -0.0038416693 | -0.1810052463 | 1.9296248881 |
| N3 | 1.8337029914 | 0.5522713932 | -0.4058329125 |
| O4 | -0.7406500067 | 2.0207228227 | 0.0557441439 |
| N5 | -0.7564536797 | -0.7860337998 | -0.9870150630 |
| Mo6 | -2.7288623733 | 2.0532838051 | -0.0838941478 |
| H7 | -1.9449753353 | -0.6707186893 | -1.3079157365 |
| C8 | -3.3659225635 | -0.4781314119 | -1.5641345731 |
| N9 | -3.2016268184 | 3.6952898914 | -0.4798820879 |
| N10 | -3.6068826250 | 0.8903201932 | -1.3864733419 |
| C11 | -3.6903007570 | -1.0944880614 | -2.8542796571 |
| Mo12 | -1.6916842046 | 0.1884485013 | 2.8499163866 |
| H13 | -3.6195979520 | -1.0656423235 | -0.6766411925 |
| O14 | -2.8460569354 | 0.9532491860 | 1.5438318652 |
| C15 | -3.7746321358 | -0.4807914911 | -4.0475923879 |
| H16 | -3.5958701364 | 0.5846561901 | -4.1751216455 |
| H17 | -4.0163344848 | -1.0351548324 | -4.9477953402 |

| | | | |
|---|---|---|---|
| H18 | -3.8392438337 | -2.1730027267 | -2.8125487784 |
| N19 | -1.4139749640 | 1.3049951859 | 4.1732563252 |
| N20 | -2.3895109835 | -1.3059386087 | 3.4538442661 |
| H21 | -0.3215259678 | -1.3326308864 | -1.7301678152 |
| H22 | -4.0358056265 | 1.3417624386 | -2.1939310951 |
| H23 | -2.6899680887 | -1.8566179012 | 4.2539377533 |
| H24 | 2.7756542390 | 0.8043029518 | -0.6819975654 |
| H25 | -3.4010894635 | 4.6220699082 | -0.1013240353 |
| H26 | -1.4529258178 | 1.5384902081 | 5.1613324082 |

**34**

Energy = -877.868749 h

Zero Point Energy (ZPE): 104.382 kcal/mol

oordinates:

| | | | |
|---|---|---|---|
| Mo1 | -0.0294586671 | -0.0245334623 | -0.0175661578 |
| O2 | 1.9196762141 | 0.0536785787 | -0.1392799381 |
| N3 | -1.0994676521 | 1.3656918749 | 0.1478843281 |
| O4 | -0.3385664529 | -1.4118973190 | 1.1996434053 |
| N5 | -0.2410963428 | -0.8249102444 | -1.8645094130 |
| Mo6 | 0.4613089064 | -3.2316883617 | 1.0481612384 |
| O7 | 2.2921865134 | -2.8640993617 | 0.6279091655 |
| Mo8 | 3.0650342109 | -1.4426549623 | -0.4617538459 |
| N9 | -0.2389496021 | -4.4308399868 | 2.1233700018 |
| N10 | -0.5295851716 | -3.6170916104 | -0.6923370802 |
| H11 | -0.3598317813 | -2.8311813428 | -1.3535353762 |
| C12 | -1.9777658683 | -4.4887650113 | -2.4305450178 |
| C13 | -1.3795557880 | -4.5096045685 | -1.1170613044 |
| H14 | 0.5349859568 | -0.6771698711 | -2.5096186808 |
| H15 | -1.6485975147 | -5.3101939237 | -0.4299985594 |
| C16 | -2.8534004800 | -5.4177214344 | -2.8567209730 |
| H17 | -3.1597568011 | -6.2430054047 | -2.2196593129 |
| H18 | -3.2851634129 | -5.3776582770 | -3.8505717619 |
| H19 | -1.6856987739 | -3.6707324281 | -3.0882120614 |
| N20 | 3.0156268268 | -1.9036090780 | -2.1666570744 |
| N21 | 4.7029964713 | -1.0849705248 | 0.0409688612 |
| H22 | -1.1203191563 | -0.6758974670 | -2.3519014145 |
| H23 | 3.5339284487 | -2.0753148039 | -3.0243567884 |
| H24 | -1.2245054924 | 2.3650797632 | -0.0035919946 |
| H25 | -0.0799212562 | -5.2201290875 | 2.7475224265 |
| H26 | 5.7059422386 | -1.0095235674 | -0.0974052666 |

**TS20**

Energy = -877.857328 h

Zero Point Energy (ZPE):101.625 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -0.0313912192 | -0.0287919886 | -0.0222080688 |
| O2 | 1.9017741014 | 0.0172435207 | -0.0517707433 |
| N3 | -1.2073938851 | 1.2887828579 | -0.0193787743 |
| O4 | -0.3165319164 | -1.4253303662 | 1.2015078513 |
| N5 | -0.2687508562 | -1.1604847470 | -1.8074786381 |
| Mo6 | 0.4777362281 | -3.2253471465 | 1.0400191281 |
| O7 | 2.3318828800 | -2.9064720131 | 0.6239012852 |
| Mo8 | 3.0700143785 | -1.4647052879 | -0.4433433282 |
| N9 | -0.1951664674 | -4.4553100392 | 2.0911832907 |
| N10 | -0.4868125148 | -3.5029298993 | -0.6970410866 |
| H11 | -0.3657165251 | -2.3798523484 | -1.3814094220 |
| C12 | -1.9350236860 | -4.3899429987 | -2.4293584221 |
| C13 | -1.3321985528 | -4.3914843153 | -1.1068687175 |
| H14 | 0.5428949653 | -1.1010980360 | -2.4286776982 |
| H15 | -1.6276268931 | -5.2021300962 | -0.4319150414 |
| C16 | -2.8259595682 | -5.3134101397 | -2.8296303980 |
| H17 | -3.1417963373 | -6.1172466795 | -2.1693942429 |
| H18 | -3.2622428812 | -5.2945098638 | -3.8225637868 |
| H19 | -1.6288030750 | -3.5970607789 | -3.1100770017 |
| N20 | 2.9169800647 | -1.8725522955 | -2.1652407628 |
| N21 | 4.7247001939 | -1.1233663333 | -0.0001130191 |
| H22 | -1.1038729914 | -0.9064415550 | -2.3325403079 |
| H23 | 3.4424490758 | -2.0115003869 | -3.0254984881 |
| H24 | -1.3382774157 | 2.2994312178 | -0.0269166351 |
| H25 | -0.0889983152 | -5.2620112588 | 2.7017438250 |
| H26 | 5.7296997822 | -1.0127817229 | -0.0820432840 |

**35**

Energy = -877.869773 h

Zero Point Energy (ZPE): 104.288 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7612388797 | 0.4809587340 | 0.7405741871 |
| O2 | -2.5301896288 | 1.9545381066 | 2.0706567014 |
| N3 | -3.4983028028 | 0.8389620170 | -0.8227267632 |
| O4 | -3.4060966978 | -0.7752741821 | 2.0752038414 |
| N5 | -0.8101183939 | -0.6180833171 | 0.6672996650 |
| Mo6 | -2.7129722622 | -1.2318570663 | 3.7892524282 |
| O7 | -1.8591426059 | 0.3363729792 | 4.4844810142 |
| Mo8 | -1.2394496283 | 1.8533587244 | 3.4316922334 |

| | | | |
|---|---|---|---|
| N9 | -3.8547708328 | -2.1974533648 | 4.7059639435 |
| N10 | -1.3364029465 | -2.4605319990 | 3.1977845013 |
| H11 | -0.8595453772 | -1.4548690827 | 1.2646747239 |
| C12 | 0.0392900785 | -4.4174789647 | 2.8538317593 |
| C13 | -1.1454553172 | -3.7280139088 | 3.3426179121 |
| H14 | -0.1337508851 | 0.0140352470 | 1.1328188095 |
| H15 | -1.8948370836 | -4.3506890787 | 3.8545074687 |
| C16 | 0.2217294076 | -5.7427248352 | 2.9891827973 |
| H17 | -0.5215690850 | -6.3679474803 | 3.4777636575 |
| H18 | 1.1129238576 | -6.2393343215 | 2.6199923932 |
| H19 | 0.7922505023 | -3.7997530113 | 2.3674645415 |
| N20 | 0.3093207822 | 1.3602802751 | 2.6368982752 |
| N21 | -1.0391166164 | 3.3072468581 | 4.3693733402 |
| H22 | -0.4684404827 | -0.8753997505 | -0.2558584857 |
| H23 | 1.2357388406 | 1.7812342650 | 2.7212706239 |
| H24 | -4.3568752862 | 0.7148878932 | -1.3585110147 |
| H25 | -4.3004555126 | -2.4725926388 | 5.5773938672 |
| H26 | -1.0305981165 | 4.1976227140 | 4.8512267693 |

**TS22**

Energy = -877.853719 h

Zero Point Energy (ZPE):101.470 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | -0.0241877212 | -0.0599756617 | 0.1341314668 |
| C2 | 1.3180805499 | -0.0398621317 | 0.0762970095 |
| C3 | 2.0672542758 | 1.2052719748 | 0.0748735416 |
| N4 | 3.3577993096 | 1.2638089366 | 0.0312792527 |
| Mo5 | 4.6245158021 | 2.8665142627 | 0.0833701597 |
| N6 | 3.6744195305 | 4.2454588197 | 0.6574874457 |
| O7 | 5.2762836452 | 3.1399252747 | -1.7160083463 |
| Mo8 | 6.6548634806 | 2.0496373941 | -2.5036456298 |
| N9 | 5.9905645770 | 0.6302094113 | -3.6740433719 |
| O10 | 7.3251833528 | 0.8554653445 | -1.1780012090 |
| Mo11 | 6.6603820165 | 0.1511619574 | 0.4852007104 |
| N12 | 7.8430857068 | -0.7249054694 | 1.4530059884 |
| N13 | 7.9709428079 | 2.9598794155 | -3.2327907002 |
| O14 | 6.0077524059 | 1.9916564098 | 0.9665105748 |
| N15 | 5.0164100545 | -0.7052181450 | 0.2750189890 |
| H16 | 4.0368774893 | 0.2192098718 | 0.0682970725 |
| H17 | 6.1965163226 | -0.3504991849 | -3.5058539691 |
| H18 | 1.4881892393 | 2.1332102036 | 0.1131726745 |
| H19 | -0.6027923601 | 0.8591555105 | 0.1830021451 |
| H20 | -0.5818860973 | -0.9905510606 | 0.1342166017 |

| | | | |
|---|---|---|---|
| H21 | 1.8891839390 | -0.9639531578 | 0.0251577665 |
| H22 | 5.5847373426 | 0.7741776044 | -4.5927530231 |
| H23 | 4.8067086426 | -1.6139101575 | 0.6910937950 |
| H24 | 3.6399164278 | 4.8834730279 | 1.4548921860 |
| H25 | 8.7997527958 | -0.6538625401 | 1.8017798890 |
| H26 | 8.7218029438 | 2.8975561502 | -3.9173079054 |

**38**

Energy = -877.878549 h

Zero Point Energy (ZPE): 102.624 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5409931167 | 0.3670727245 | 0.6499718141 |
| O2 | -1.6372784443 | 1.5114057586 | 1.8735142165 |
| N3 | -3.5222566835 | 1.2423327406 | -0.5129344780 |
| O4 | -3.5715463269 | -0.4485744025 | 2.0492713335 |
| N5 | -1.3712768712 | -0.8908729678 | -0.2527578874 |
| Mo6 | -3.1670894454 | -1.1111262293 | 3.8108167442 |
| O7 | -1.9608895285 | 0.1487735576 | 4.6677033913 |
| Mo8 | -1.0286451216 | 1.5144605634 | 3.7074420657 |
| N9 | -4.6119964069 | -1.4707392291 | 4.7223375443 |
| N10 | -2.2397265618 | -2.6948620390 | 3.4563684262 |
| H11 | 1.1586950878 | 1.1608293522 | 2.2722890820 |
| C12 | -0.9643937065 | -4.7086320972 | 3.0830242682 |
| C13 | -2.1536098280 | -3.9862215384 | 3.4839997705 |
| H14 | -0.6996284164 | -1.4980204006 | 0.2072583452 |
| H15 | -3.0087184126 | -4.5855822017 | 3.8274599965 |
| C16 | -0.8744322264 | -6.0534686315 | 3.1047552161 |
| H17 | -1.7070217979 | -6.6722400486 | 3.4297860083 |
| H18 | 0.0298955447 | -6.5696586101 | 2.8004054111 |
| H19 | -0.1212907868 | -4.1018910346 | 2.7586411770 |
| N20 | 0.8202821521 | 1.0750361101 | 3.2266134007 |
| N21 | -1.1585894794 | 3.1033290440 | 4.4438518160 |
| H22 | -1.3770079386 | -1.0241904126 | -1.2585166615 |
| H23 | 1.5889197325 | 1.0192770297 | 3.8865583874 |
| H24 | -4.2512439445 | 1.9575466916 | -0.4853845511 |
| H25 | -5.3726182776 | -1.9608300721 | 5.1802737316 |
| H26 | -0.7583824645 | 4.0360497343 | 4.5129229777 |

**TS21**

Energy = -877.815851

Zero Point Energy (ZPE): 102.017 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.2906857571 | -0.5777395000 | 0.1571585354 |
| C2 | 0.1845485812 | -0.1028068943 | 1.4060434639 |
| C3 | 1.3100818797 | -0.0260951199 | 2.3473516950 |
| N4 | 1.1321825353 | 0.2247647155 | 3.5837186692 |
| Mo5 | 2.8507299027 | -0.3370828446 | 4.3852687219 |
| N6 | 2.5448139261 | -0.8790996553 | 6.0342373747 |
| O7 | 4.0517662632 | 1.2234202333 | 4.5823466806 |
| Mo8 | 5.3739343003 | 2.1343159642 | 3.6130652926 |
| N9 | 4.7207153683 | 2.8447346365 | 1.6237440476 |
| O10 | 6.1453872700 | 0.6466855244 | 2.5037563874 |
| Mo11 | 5.1353278949 | -0.7448681827 | 1.8247241720 |
| N12 | 6.0472554905 | -1.8205874936 | 0.7730402098 |
| N13 | 6.5990221976 | 3.2824558089 | 4.1299820270 |
| O14 | 4.0812439900 | -1.3659194813 | 3.2514949404 |
| N15 | 3.6448151101 | 0.1024954924 | 0.9353343385 |
| H16 | 4.1830009675 | 3.7069456726 | 1.5866329240 |
| H17 | 4.1602872934 | 2.0620154812 | 1.2362985568 |
| H18 | 2.6253555515 | -0.0187656383 | 1.5734183445 |
| H19 | 1.2370885664 | -0.9374592671 | -0.2363705578 |
| H20 | -0.5723047594 | -0.6456060565 | -0.4978204693 |
| H21 | -0.7809040155 | 0.2248815944 | 1.7936842318 |
| H22 | 5.5343072395 | 2.9445473364 | 1.0174540006 |
| H23 | 3.4471785669 | -0.0400111573 | -0.0548662535 |
| H24 | 7.0854698491 | 3.7912494148 | 4.8647427914 |
| H25 | 3.0022582943 | -1.5603598574 | 6.6485786302 |
| H26 | 6.3492241950 | -2.7528350739 | 0.5028048590 |

**TS23**

Energy = -877.827816 hartrees

Zero Point Energy (ZPE): 101.431 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.2352623871 | 0.5059887973 | -0.0334061457 |
| C2 | 0.4915027022 | 0.5701395245 | 1.2811653769 |
| C3 | 1.5153612169 | -0.2776526388 | 1.9015566149 |
| N4 | 1.7459611525 | -0.2581261745 | 3.1413553666 |
| Mo5 | 2.7969129984 | -0.3214798580 | 4.7123058436 |
| N6 | 2.0199937250 | -1.2099809603 | 6.0261024483 |
| O7 | 3.7825119105 | 1.3181211151 | 4.8276729341 |
| Mo8 | 4.9097877107 | 2.1517136060 | 3.5192603840 |
| N9 | 3.4255555247 | 3.2131055942 | 2.8031972895 |
| O10 | 5.5905005698 | 0.8189898647 | 2.2970148834 |
| Mo11 | 5.2487521597 | -1.0856435831 | 2.4631857017 |
| N12 | 6.4493219678 | -2.3190485617 | 2.0810690386 |
| N13 | 6.1346194226 | 3.1340547888 | 4.2990219068 |

| | | | |
|---|---|---|---|
| O14 | 4.4715021368 | -1.2807091519 | 4.1338416648 |
| N15 | 3.8405339981 | -1.1484308044 | 0.8353022807 |
| H16 | 2.5248335287 | 3.2586683276 | 3.2727534692 |
| H17 | 4.0672087435 | -0.4593679205 | 0.1161082384 |
| H18 | 2.7041320485 | -0.8838928595 | 1.2045981319 |
| H19 | 0.7792764156 | -0.1785380125 | -0.6787827772 |
| H20 | -0.5272220862 | 1.1237593694 | -0.4981076789 |
| H21 | -0.0711739751 | 1.2489259071 | 1.9240804681 |
| H22 | 3.5244078122 | 3.9581015087 | 2.1214034086 |
| H23 | 3.8031351773 | -2.0606623065 | 0.3820284770 |
| H24 | 7.3059893132 | -2.4690603540 | 1.5470947831 |
| H25 | 6.3834909291 | 4.0049101564 | 4.7609833758 |
| H26 | 2.0836762176 | -1.3134786297 | 7.0395080846 |

**36**

Energy = -877.851039 h

Zero Point Energy (ZPE): 105.091 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6906640450 | 0.3473930499 | 0.7705880805 |
| O2 | -2.1207213582 | 1.9373180902 | 1.7973045048 |
| N3 | -3.3885433827 | 0.7452285964 | -0.8056840121 |
| O4 | -3.4610674565 | -0.7462669946 | 2.0504947102 |
| N5 | -0.7933845357 | -0.4488949150 | 0.5333630237 |
| Mo6 | -2.9626175138 | -1.2218715318 | 3.9359830729 |
| O7 | -2.0148094141 | 0.3025252019 | 4.3683394245 |
| Mo8 | -1.1643924502 | 1.8701311595 | 3.4243441938 |
| N9 | -4.3348338263 | -1.8733449314 | 4.8403761797 |
| N10 | -1.8920518504 | -2.8818033886 | 3.4033608819 |
| H11 | 0.1657185967 | 0.0030754510 | 2.1210393184 |
| C12 | -0.7752585103 | -5.1634644510 | 2.9335547900 |
| C13 | -1.3885530040 | -3.9207825841 | 3.1794071413 |
| H14 | -0.2687986268 | 0.0574058993 | -0.1807334234 |
| H15 | 0.5053009292 | -0.2711695528 | 3.7457041119 |
| C16 | -1.3128144027 | -6.3539255544 | 3.2775051328 |
| H17 | -2.2703802171 | -6.4270187329 | 3.7807789787 |
| H18 | -0.7897182293 | -7.2750087630 | 3.0495163692 |
| H19 | 0.1856490339 | -5.1108904758 | 2.4259316073 |
| N20 | 0.4590732928 | 0.4517960165 | 3.0249520720 |
| N21 | -0.5480397766 | 3.0997207984 | 4.5341521369 |
| H22 | -0.7937464519 | -1.4266828149 | 0.2425178240 |
| H23 | 1.3836841819 | 0.8590654687 | 2.9115711258 |
| H24 | -4.2037201720 | 0.5754618802 | -1.3932120044 |
| H25 | -4.8320213009 | -1.7879798079 | 5.7269583069 |
| H26 | -0.4557633862 | 4.0990411218 | 4.7115407645 |

**37** (one Mo-Mo bond)
Energy = -707.014320 h
Zero Point Energy (ZPE): 72.446 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.4871321924 | 0.2404514344 | 0.7363753307 |
| O2 | -1.7033788407 | 1.6658408889 | 1.7566293818 |
| N3 | -3.4245022593 | 0.6513277888 | -0.6873885967 |
| O4 | -3.2591511070 | -1.0816629094 | 1.9034920358 |
| N5 | -0.6270888640 | -0.3063095228 | 0.1651075643 |
| Mo6 | -3.1520748280 | -0.7073463946 | 3.8094127724 |
| O7 | -1.3246667962 | -0.4693231485 | 4.3643546930 |
| Mo8 | -1.3632248905 | 1.3532386090 | 3.6464924821 |
| N9 | -4.3598141320 | -0.2839927377 | 5.0040135056 |
| H10 | 0.5395074864 | 0.2073406315 | 2.0984584420 |
| H11 | -0.0379310620 | 0.4550224965 | -0.1702008149 |
| H12 | 1.1500417094 | 0.1265912910 | 3.6399724809 |
| N13 | 0.7296218845 | 0.7495214440 | 2.9528510080 |
| N14 | -1.5579454903 | 2.6287737665 | 4.8375712113 |
| H15 | -0.5422222902 | -1.0785252730 | -0.4925268657 |
| H16 | 1.3872896121 | 1.4910810607 | 2.7252057287 |
| H17 | -5.2569549455 | -0.0373077739 | 5.4113416765 |
| H18 | -1.7084881527 | 3.6280631112 | 4.9627242396 |
| H19 | -3.5972553732 | 1.2443166958 | -1.4948273077 |

**37** (two Mo-Mo bonds)
Energy = -707.034842 hartrees
Zero Point Energy (ZPE): 72.529 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.7142727717 | 0.0785705286 | 1.1741411711 |
| O2 | -1.1723108602 | 1.2748947712 | 1.5325967493 |
| N3 | -4.1885498215 | 0.8361679371 | 0.5997506520 |
| O4 | -2.6023379234 | -1.6444114222 | 2.0992235545 |
| N5 | -1.3821037098 | -0.9513881685 | -0.3978316671 |
| Mo6 | -2.7245403911 | -0.6308751749 | 3.7459017017 |
| O7 | -1.0130434829 | -0.1719672560 | 4.4970339077 |
| Mo8 | -1.1044431891 | 1.4732332979 | 3.4331694842 |
| N9 | -4.1767772640 | -0.0635775374 | 4.5626241764 |
| H11 | -1.7195829868 | -0.9237870212 | -1.3567591459 |
| H15 | 1.1469743731 | 2.6088812437 | 4.2349021648 |
| N20 | 0.7675789887 | 1.6906949010 | 4.0289519253 |
| N21 | -2.0047740773 | 2.8699813513 | 4.0009310918 |
| H23 | 1.2292979944 | 0.9710211636 | 4.5768834406 |

| | | | |
|---|---|---|---|
| H24 | -5.1938521619 | 0.8439816272 | 0.4490448118 |
| H25 | -5.1902604645 | 0.0075580799 | 4.6066718124 |
| H26 | -2.4154149181 | 3.2989202451 | 4.8289630134 |
| H18 | -0.4730861554 | -0.4911160209 | -0.3624294700 |
| H19 | -1.2669692641 | -1.9238368418 | -0.1158842409 |

**39**

Energy = -876.636833 h

Zero Point Energy (ZPE): 87.896 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.6267096389 | 0.3325868589 | 0.6815404995 |
| O2 | -2.2457006418 | 1.8371719185 | 1.8032983913 |
| N3 | -3.8336978731 | 0.5368075548 | -0.6032216946 |
| O4 | -3.2677125706 | -0.9337720969 | 2.0038821174 |
| N5 | -1.2043977237 | -0.3572887003 | -0.1381750514 |
| Mo6 | -2.4420798154 | -1.2597962829 | 3.7044495805 |
| O7 | -2.1152851861 | 0.4557692562 | 4.5275513854 |
| Mo8 | -1.5093801509 | 2.0268632238 | 3.5827363659 |
| N9 | -3.3681478273 | -2.3698473825 | 4.6812602258 |
| N10 | -0.7836183750 | -1.9821179017 | 3.2380641703 |
| H11 | -0.3333199751 | -0.5222023419 | 0.3831613408 |
| C12 | -0.0669036607 | -4.2861582772 | 3.5883808764 |
| C13 | 0.1152207420 | -2.9096597081 | 3.1767813515 |
| H14 | 1.1002841282 | -2.6406219657 | 2.7747046620 |
| C15 | 0.9159086118 | -5.2024335552 | 3.4946534251 |
| H16 | 1.8967055277 | -4.9420903090 | 3.1044549557 |
| H17 | 0.7680626821 | -6.2322763947 | 3.8016479516 |
| H18 | -1.0468802785 | -4.5538861331 | 3.9767102091 |
| N19 | 0.2421287845 | 2.0712131816 | 3.5096968099 |
| N20 | -2.1233109150 | 3.4670162987 | 4.3657049511 |
| H21 | 1.1292160579 | 2.5326812101 | 3.6932404466 |
| H22 | -4.7224961596 | 1.0363070451 | -0.4846974710 |
| H23 | -3.6777589749 | -3.1931688134 | 5.1865622596 |
| H24 | -1.9583918950 | 4.3733190988 | 4.7957682420 |

**TS24**

Energy = -876.611537 hartrees

Zero Point Energy (ZPE): 85.921 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| C1 | 0.0124677123 | -0.0806907751 | 0.0254627448 |
| C2 | 1.3332439298 | 0.1342867460 | 0.1024086830 |
| C3 | 1.9506159460 | 1.3036642874 | -0.5219975381 |

| | | | |
|---|---|---|---|
| N4 | 3.1656069530 | 1.6018943059 | -0.4605577811 |
| Mo5 | 4.4957720410 | 2.9730878167 | -0.5113611374 |
| N6 | 5.7343910547 | 2.5025488391 | -1.6635926905 |
| O7 | 4.5014531956 | 3.7281856737 | 1.3039192057 |
| Mo8 | 3.4664047209 | 5.0680102717 | 2.1724438502 |
| N9 | 2.7689897247 | 4.3934341859 | 3.6364091627 |
| O10 | 2.0214016037 | 5.6336743601 | 0.9769041481 |
| Mo11 | 1.9407325106 | 5.1568998816 | -0.8621480480 |
| N12 | 1.3922648751 | 6.4367878651 | -1.9049223265 |
| N13 | 4.4827879503 | 6.4358009028 | 2.5804668148 |
| O14 | 3.7064209485 | 4.7027181029 | -1.1883651865 |
| N15 | 0.8155662981 | 3.6578822249 | -1.0660853815 |
| H16 | 2.6543796214 | 4.4507929652 | 4.6447987460 |
| H17 | 1.2002154972 | 2.5239639856 | -0.9292986937 |
| H18 | -0.6394206427 | 0.6063632622 | -0.5063408152 |
| H19 | -0.4514268340 | -0.9434779321 | 0.4935020641 |
| H20 | 1.9822127999 | -0.5587885496 | 0.6381810454 |
| H21 | -0.0246594141 | 3.6681882057 | -1.6424822171 |
| H22 | 6.7105362590 | 2.5242991544 | -1.9545247755 |
| H23 | 1.2445004725 | 7.2794105016 | -2.4487007367 |
| H24 | 4.8697245289 | 7.0777158844 | 3.2663048877 |

**40**

Energy = -876.624319 hartrees
Zero Point Energy (ZPE): 88.754 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.4302379537 | 0.2327765120 | 0.7371140635 |
| O2 | -2.1164423743 | 1.8489608208 | 1.8499208764 |
| N3 | -3.3342373494 | 0.5808954362 | -0.7620858593 |
| O4 | -3.2880136279 | -0.7475676644 | 2.0783683562 |
| N5 | -0.8059853330 | -0.3365908752 | 0.2415705289 |
| Mo6 | -2.9981884997 | -1.1855214370 | 3.9794056147 |
| O7 | -1.9414996202 | 0.2911476931 | 4.5048619269 |
| Mo8 | -1.2238903826 | 1.8177390163 | 3.5062120847 |
| N9 | -4.5172713678 | -1.6294552031 | 4.7163788670 |
| N10 | -2.1671524294 | -3.0019966177 | 3.5112595700 |
| H11 | -0.1335971492 | -0.6339214951 | 0.9617154780 |
| C12 | -1.1719631458 | -5.3041393530 | 2.8941736626 |
| C13 | -1.7216653577 | -4.0460504568 | 3.2256905358 |
| H15 | 1.3733841303 | 1.3190604963 | 3.3929579330 |
| C16 | -1.7492151067 | -6.4746018757 | 3.2261970849 |
| H17 | -2.6785746694 | -6.5199748074 | 3.7833754272 |
| H18 | -1.2913067418 | -7.4116794633 | 2.9319084305 |
| H19 | -0.2421206578 | -5.2664679093 | 2.3318433202 |

| | | | |
|---|---|---|---|
| N20 | 0.5541840277 | 1.2984891132 | 2.7927473026 |
| N21 | -1.0182127872 | 3.2444236061 | 4.5161023923 |
| H23 | 0.7957906293 | 1.6514518012 | 1.8675668175 |
| H24 | -4.3416115024 | 0.7829199612 | -0.7282594769 |
| H25 | -5.2919940349 | -1.5097629936 | 5.3636977625 |
| H26 | -1.0023611522 | 4.2616946397 | 4.5605321964 |

**41**

Energy = -705.797843 hartrees

Zero Point Energy (ZPE): 56.538 kcal/mol

Coordinates:

| | | | |
|---|---|---|---|
| Mo1 | -2.5615583305 | -0.0012584656 | 0.7961990711 |
| O2 | -1.4942758450 | 1.4393732302 | 1.5695967474 |
| N3 | -4.0617672720 | 0.6412658471 | 0.1546626991 |
| O4 | -2.9355923403 | -1.3756111850 | 2.1186542108 |
| N5 | -1.6302227715 | -0.7266120907 | -0.4966786832 |
| Mo6 | -2.8147229622 | -0.6756105742 | 3.9015944613 |
| O7 | -1.0759826133 | -0.0992618801 | 4.5231470877 |
| Mo8 | -1.1647698631 | 1.5062736681 | 3.4456426222 |
| N9 | -4.1324294502 | -0.1137521409 | 4.9058783533 |
| H11 | -1.4705272582 | -0.9978424495 | -1.4627211482 |
| H15 | 1.1713015458 | 2.6043179817 | 4.0289671431 |
| N20 | 0.7670505111 | 1.7240716164 | 3.7280281750 |
| N21 | -2.0159612009 | 2.7976491255 | 4.2228529891 |
| H23 | 1.3659588869 | 0.9422154627 | 3.9787166036 |
| H24 | -4.6597640551 | 0.8143835205 | -0.6495053521 |
| H25 | -5.1076832900 | 0.1008546245 | 5.0985840941 |
| H26 | -2.6275283136 | 3.4513231260 | 4.6971594308 |

## Detailed discussion of ammoxidation pathways for the intermediate feed pressures with cluster model with three NH groups (Figure 9).

The **TS13** leads to the intermediate **24** with a Mo-(NH=CH-CH=$CH_2$) fragment and Mo-$NH_2$ and Mo=NH sites. The net barrier for the third hydrogen abstraction on **Path 1b** through **TS14** is 5.0 kcal/mol ($\Delta G^{\ddagger}_{673K}$ = 0.2 kcal/mol) lower than the corresponding barrier on **Path 2b** through **TS16**. The product on **Path 1b** (**25**) with $Mo^{IV}$-$NH_3$ and $Mo^{VI}$=NH sites is 7.9 kcal/mol ($\Delta G_{673K}$ = 17.1 kcal/mol) less stable than the product on **Path 2b** (**28**) with two $Mo^{V}$-$NH_2$ sites. This order is reversed in a case of corresponding products at low partial pressures (**Error! Reference source not found.**). The barrier for the last hydrogen abstraction is higher than for previous steps for both pathways, as it leads to reduction of all three molybdenum centers to unfavorable $Mo^{IV}$ and $Mo^{V}$ states. Our calculated net barrier on **Path 1b** (**TS15**) is $\Delta E^{\ddagger}$ = 35.0 kcal/mol ($\Delta G^{\ddagger}_{673K}$ = 32.8 kcal/mol), and the net barrier for on **Path 2b** (**TS17**) is $\Delta E^{\ddagger}$ = 36.8 kcal/mol ($\Delta G^{\ddagger}_{673K}$ = 42.7 kcal/mol). This step is feasible on **Path 1b** at the 400°C reaction temperature, but the barriers are higher than the barrier for the second hydrogen abstraction ($\Delta E^{\ddagger}$ = 25.9 kcal/mol and $\Delta G^{\ddagger}_{673K}$ = 29.7 kcal/mol for **TS13**), therefore, below we consider the effect of fully oxidized sites on **TS15** barrier, as already described for similar cases in the previous sections.

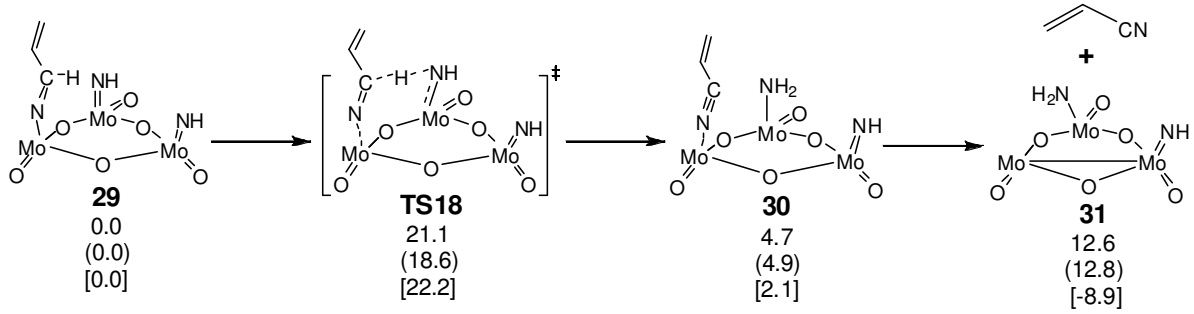
The product **26** with $Mo^{IV}$-$NH_3$, $Mo^{V}$-$NH_2$, and acrylonitrile coordinated to $Mo^{IV}$ is more stable than the corresponding product **15**, as the energy cost for breaking Mo=O bond is higher than for Mo=NH bond. Energy cost for dissociation of acrylonitrile from **26** to give **27** with a Mo-Mo bond between a vacant Mo and Mo-$NH_3$ ($R_{Mo\text{-}Mo}$ = 2.78 Å) is 17.2 kcal/mol ($\Delta G_{673K}$ = -6.3 kcal/mol). In the case of isomer with two Mo-Mo bonds ($R_{Mo\text{-}Mo\text{-}NH3}$ = 2.68 Å, and ($R_{Mo\text{-}Mo\text{-}NH2}$ = 2.70 Å), the desorption energy is $\Delta E$ = -2.5 kcal/mol ($\Delta G_{673K}$ = -24.8 kcal/mol), and for the case with no Mo-Mo bonds, the desorption energy is $\Delta E$ = 22.6 kcal/mol ($\Delta G_{673K}$ = 3.6 kcal/mol).

*Product Formation on Re-oxidized Cluster*

To verify that the fourth hydrogen abstraction barrier decreases in presence of re-oxidized active surface sites, we considered this step using the $Mo_3O_6(NH)_2$(N=CH-CH=$CH_2$) cluster (**29**), which has two fully oxidized molybdenum centers, $Mo^{VI}$=NH, where the $Mo^{IV}$-$NH_3$ in **25** is replaced by a $Mo^{VI}$=NH via ammonia activation process. Energetics for this pathway are given in

**Scheme** 1. The barrier for the last H abstraction through **TS18** is 21.1 kcal/mol ($\Delta G^{\ddagger}_{673K}$ = 22.2 kcal/mol), which is 13.9 kcal/mol lower than the **TS15** barrier. In addition it is 9.6 kcal/mol lower than the corresponding barrier at low partial pressures of feed (**TS6** in **Error! Reference source not found.**), and 3.5 kcal/mol lower than the corresponding barrier at intermediate pressures with two imido-oxo and one oxo-oxo sites (**TS12**). According to our calculations, re-oxidation of reduced sites prior to fourth

hydrogen abstraction might further contribute to higher conversion rates for intermediate feed pressures.




**Scheme 1**. Fourth hydrogen abstraction in conversion of allyl to acrylonitrile over re-oxidized cluster (intermediate feed pressures). The barrier is significantly reduced compared to the barrier on the reduced site (TS15) making this process more rapid at reaction temperature. The top energy parameter is the ΔE from QM, the middle is $\Delta H_{0K}$ = ΔE+ΔZPE, and the bottom is $\Delta G_{673K}$. All reported values are in kcal/mol.

In **TS18** the breaking and forming C-H and N-H distances are 1.45 Å and 1.23 Å, respectively. The transition state normal mode has an imaginary frequency of 1334i $cm^{-1}$. Product **30** is more stable than corresponding **20**, with abstraction energy ΔE = 4.7 kcal/mol ($\Delta G_{673K}$ = 2.1 kcal/mol). The Mo-(NC-CH=$CH_2$) distance is 2.05 Å and the Mo-N-C angle is 176 degrees.

Desorption of acrylonitrile from **30** to give $Mo_3O_6(NH)(NH_2)$ (**31**) with one Mo-Mo bond between a vacant Mo and Mo-$NH_2$ has desorption energy ΔE = 7.9 kcal/mol ($\Delta G_{673K}$ = -11.0 kcal/mol). For the case of reduced cluster with no Mo-Mo bonds, the desorption energy is ΔE = 18.4 kcal/mol ($\Delta G_{673K}$ = -6.2 kcal/mol).